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INTRODUCTION TO INTEGRABLE MANY-BODY SYSTEMS III

Zoltán Bajnok[1]
Theoretical Physics Research Group, Hungarian Academy of Sciences, Eötvös University, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary

Ladislav Šamaj[2]
Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia

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This is the third part of a three-volume introductory course about integrable systems of interacting bodies. The emphasis is put onto the method of Thermodynamic Bethe ansatz. Two kinds of integrable models are studied. Systems of itinerant electrons, forming a part of Condensed Matter Physics, involve the Hubbard lattice model of electrons with short-ranged one-site interactions (Sect. 20) and the s-d exchange Kondo model (Sect. 21), describing the scattering of conduction electrons on a spin-s impurity. Methods and basic concepts used in Quantum Field Theory are explained on the integrable $(1+1)$-dimensional sine-Gordon model. We start with the classical description of the model in Sect. 22, analyze its finite energy field configurations (soliton, anti-soliton and breathers) and show its classical integrability. The model is quantized by using two schemes: the conformal (Sect. 23) and Lagrangian (Sect. 24) quantizations. The scattering matrix of the sine-Gordon theory is derived at the full quantum level in the bootstrap scheme and is compared to its classical limit in Sect. 25. The parameters of the scattering matrix are related to those of the Lagrangian by calculating the ground-state energy in an applied magnetic field in two ways: Conformal perturbation theory and Thermodynamic Bethe ansatz (Sect. 26). The relation of the sine-Gordon theory to the XXZ Heisenberg model, which provides a complete solution of the sine-Gordon model in a finite volume, is pointed out in Sect. 27. The obtained results are applied in Sect. 28. to the derivation of the exact thermodynamics for the (symmetric) two-component Coulomb gas; this is the first classical two-dimensional fluid with exactly solvable thermodynamics.

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[1]E-mail address: bajnok@elte.hu
[2]E-mail address: Ladislav.Samaj@savba.sk

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CONDENSED MATTER: MODELS OF ITINERANT ELECTRONS

20 Hubbard model

The Hubbard model [1] has long been the most important model system of strongly interacting electrons in a solid. It is investigated in connection with the metal-insulator transition of Mott type [2]. This model represents a lattice version of the spin-$\frac{1}{2}$ fermion gas with δ-function pair interactions, studied in Sect. 10. The 1D Hubbard model was solved using the Bethe ansatz by Lieb and Wu [3]; for a reminiscence and some new rigorous results, see Ref. [4]. The topic has been summarized in the monograph [5].

20.1 Hamiltonian and its symmetries

We start with a general set-up for electrons with spin $\sigma \in \{\uparrow, \downarrow\}$, formulated on a periodic chain of atomic sites $l = 1, 2, \ldots, L$. In the framework of the second quantization, let $c^\dagger_{l\sigma}$ and $c_{l\sigma}$ be creation and annihilation operators of an electron of spin σ at site l, satisfying the usual anticommutation relations

$$\{c_{l\sigma}, c_{l'\sigma'}\} = \{c^\dagger_{l\sigma}, c^\dagger_{l'\sigma'}\} = 0, \qquad \{c^\dagger_{l\sigma}, c_{l'\sigma'}\} = \delta_{ll'}\delta_{\sigma\sigma'}. \tag{20.1}$$

The chain periodicity is ensured by setting $c_{L+1\sigma} = c_{1\sigma}$. For electrons with spin $\sigma \in \{\uparrow, \downarrow\}$, we define the local occupation number operator $n_{l\sigma} = c^\dagger_{l\sigma} c_{l\sigma}$ and the total number operator $\hat{N}_\sigma = \sum_l n_{l\sigma}$. The number operator of all electrons is $\hat{N} = \hat{N}_\uparrow + \hat{N}_\downarrow$. The operators of the components of the total spin are defined as follows

$$S^\alpha_{\rm tot} = \frac{1}{2} \sum_{l=1}^{L} \sum_{\sigma', \sigma''=\uparrow,\downarrow} c^\dagger_{l\sigma'} \, (\sigma^\alpha)^{\sigma'}_{\sigma''} \, c_{l\sigma''}, \qquad \alpha = x, y, z, \tag{20.2}$$

where $\{\sigma^\alpha\}$ are the usual Pauli matrices. Explicitly, we have

$$\begin{aligned} S^x_{\rm tot} &\equiv \frac{1}{2} \sum_l \left(c^\dagger_{l\uparrow} c_{l\downarrow} + c^\dagger_{l\downarrow} c_{l\uparrow} \right), \\ S^y_{\rm tot} &\equiv \frac{1}{2\mathrm{i}} \sum_l \left(c^\dagger_{l\uparrow} c_{l\downarrow} - c^\dagger_{l\downarrow} c_{l\uparrow} \right), \\ S^z_{\rm tot} &\equiv \frac{1}{2} \sum_l \left(c^\dagger_{l\uparrow} c_{l\uparrow} - c^\dagger_{l\downarrow} c_{l\downarrow} \right). \end{aligned} \tag{20.3}$$

The spin operators generate a representation of su(2) algebra, $[S^\alpha_{\rm tot}, S^\beta_{\rm tot}] = \mathrm{i}\epsilon_{\alpha\beta\gamma} S^\gamma_{\rm tot}$. It is useful to introduce the ladder operators $S^\pm_{\rm tot} = S^x_{\rm tot} \pm \mathrm{i} S^y_{\rm tot}$, which have the explicit forms

$$S^+ = \sum_l c^\dagger_{l\uparrow} c_{l\downarrow}, \qquad S^- = \sum_l c^\dagger_{l\downarrow} c_{l\uparrow}. \tag{20.4}$$

They obey the sl(2) commutation relations

$$\left[S^+_{\rm tot}, S^-_{\rm tot}\right] = 2S^z_{\rm tot}, \qquad \left[S^z_{\rm tot}, S^\pm_{\rm tot}\right] = \pm S^\pm_{\rm tot}. \tag{20.5}$$

The vacuum state vector $|0\rangle$, corresponding to the empty lattice, is defined by

$$c_{l\sigma}|0\rangle = 0 \qquad \text{for } l = 1, \ldots, L \text{ and } \sigma = \uparrow, \downarrow. \tag{20.6}$$

The basis of the space of states is generated by applying the creation operators $\{c^\dagger_{l\sigma}\}$ to $|0\rangle$. For N electrons, we introduce the ordered coordinates $\mathbf{l} = (l_1, \ldots, l_N)$ with $l_j \leq l_{j+1}$ and spin components $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$ such that $\sigma_j < \sigma_{j+1}$ if $l_j = l_{j+1}$. The space of states is spanned by all linear combination of Wannier states:

$$|\mathbf{l}, \boldsymbol{\sigma}\rangle = c^\dagger_{l_N \sigma_N} \ldots c^\dagger_{l_1 \sigma_1}|0\rangle. \tag{20.7}$$

For $N_\uparrow$ electrons with spin up and $N_\downarrow$ electrons with spin down, the total number of Wannier states is $\binom{L}{N_\uparrow}\binom{L}{N_\downarrow}$. Thus, the dimension of the Wannier space is

$$\sum_{N_\uparrow=0}^{L} \sum_{N_\downarrow=0}^{L} \binom{L}{N_\uparrow}\binom{L}{N_\downarrow} = 4^L. \tag{20.8}$$

The same number can be obtained directly by noting that each atomic site $l = 1, \ldots, L$ has four states, namely the empty state $|0\rangle$, the spin-up state $c^\dagger_{l\uparrow}|0\rangle$, the spin-down state $c^\dagger_{l\downarrow}|0\rangle$ and the fully occupied spin-up plus spin-down state $c^\dagger_{l\uparrow}c^\dagger_{l\downarrow}|0\rangle$; due to the Pauli exclusion principle, electrons of the same spin cannot occupy the same site.

The one-body kinetic energy of electrons T is composed of nearest-neighbour hopping terms,

$$T = -t\sum_{l=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{l\sigma}c_{l+1\sigma} + c^\dagger_{l+1\sigma}c_{l\sigma}). \tag{20.9}$$

In what follows, energies will be measured in units of $t = 1$. The interaction energy of electrons V is approximated by only short-range contributions from sites doubly occupied by electrons with opposite spins,

$$V = 2c\sum_{l=1}^{L} n_{l\uparrow}n_{l\downarrow}. \tag{20.10}$$

Since the electrons possess the same charge, the usual version of the Hubbard model corresponds to the repulsive Coulomb coupling constant $c > 0$. However, instead of electrons we can consider the spinless fermions which are distinguished by the charge (two-component plasma), so that the Coulomb attraction between a $+$ charge and $-$ charge at the same site leads to the attractive Hubbard model with $c < 0$. The Hubbard Hamiltonian is given by $H \equiv H(c) = T + V$.

Now we show that the numbers of up-spin electrons $\hat{N}_\uparrow = \sum_l n_{l\uparrow}$ and down-spin electrons $\hat{N}_\downarrow = \sum_l n_{l\downarrow}$ are conserved, i.e.

$$\left[H, \hat{N}_\sigma\right] = 0, \qquad \sigma = \uparrow, \downarrow, \tag{20.11}$$

together with the obvious relation $[\hat{N}_\uparrow, \hat{N}_\downarrow] = 0$. With regard to (20.1), the local occupation number operators satisfy the relations

$$\left[n_{l\sigma}, c^\dagger_{k\sigma'}\right] = \delta_{lk}\delta_{\sigma\sigma'}c^\dagger_{k\sigma'}. \tag{20.12}$$

The summation of this equation over $l = 1, \ldots, L$ leads to a couple of the Hermitian conjugate equations

$$\left[\hat{N}_\sigma, c^\dagger_{l\sigma'}\right] = \delta_{\sigma\sigma'} c^\dagger_{l\sigma'}, \qquad \left[\hat{N}_\sigma, c_{l\sigma'}\right] = -\delta_{\sigma\sigma'} c_{l\sigma'}. \tag{20.13}$$

Consequently,

$$\left[\hat{N}_\sigma, c^\dagger_{l\sigma'} c_{k\sigma'}\right] = \left[\hat{N}_\sigma, c^\dagger_{l\sigma'}\right] c_{k\sigma'} + c^\dagger_{l\sigma'} \left[\hat{N}_\sigma, c_{k\sigma'}\right] = 0. \tag{20.14}$$

This equality implies immediately the conservation laws (20.11). Since the total number of electrons is given by $\hat{N} = \hat{N}_\uparrow + \hat{N}_\downarrow$ and the z-component of the total spin by $S^z_{\rm tot} = (\hat{N}_\uparrow - \hat{N}_\downarrow)/2$, these quantities are conserved as well,

$$\left[H, \hat{N}\right] = [H, S^z_{\rm tot}] = 0. \tag{20.15}$$

In the canonical approach, we fix the numbers $N_\uparrow$ of up-spin electrons and $N_\downarrow$ of down-spin electrons. In the grand-canonical formalism, the control variables are the external magnetic field $h \geq 0$ (hence $n_\uparrow \geq n_\downarrow$) and the chemical potential μ of particles. The Hamiltonian then reads

$$H(c, h) = H(c) - 2hS^z_{\rm tot}. \tag{20.16}$$

Due to the conservation laws (20.15), the Hamiltonians $H(c)$ and $H(c, h)$ possess the common set of eigenstates.

For a bipartite chain with $L =$ even number of sites, the set of lattice sites can be divided into two subsets, $A = \{1, 3, 5, \ldots\}$ and $B = \{2, 4, 6, \ldots\}$, such that there is no hopping between A sites or B sites. Then, the unitary transformation $U^\dagger H U$ with $U = \exp[\mathrm{i}\pi \sum_{l\in A}(n_{l\uparrow} + n_{l\downarrow})]$ leaves H unchanged, except for the replacement $T \to -T$.

For the bipartite chain, the 1D Hubbard model possesses many symmetries based on the particle-hole transformations. Let us first introduce the "hole" fermion operators

$$\begin{array}{lll} a^\dagger_{l\sigma} = c_{l\sigma}, & a_{l\sigma} = c^\dagger_{l\sigma}, & \text{for } l \in A \text{ and } \sigma \in \{\uparrow, \downarrow\}, \\ a^\dagger_{l\sigma} = -c_{l\sigma}, & a_{l\sigma} = -c^\dagger_{l\sigma}, & \text{for } l \in B \text{ and } \sigma \in \{\uparrow, \downarrow\}. \end{array} \tag{20.17}$$

Under this transformation, the Hamiltonian (20.16) and the particle numbers are changed to

$$H(c, h) \to 2c(L - \hat{N}) + H(c, -h), \qquad \hat{N}_\uparrow \to L - \hat{N}_\uparrow, \quad \hat{N}_\downarrow \to L - \hat{N}_\downarrow. \tag{20.18}$$

In this way the more than half-filled case $(N > L)$ is mapped onto the less than half-filled case $(N < L)$. If the transformation (20.17) is made only for spin-up electrons, i.e.

$$\begin{array}{lll} a^\dagger_{l\uparrow} = c_{l\uparrow}, & a_{l\uparrow} = c^\dagger_{l\uparrow}, & \text{for } l \in A, \\ a^\dagger_{l\uparrow} = -c_{l\uparrow}, & a_{l\uparrow} = -c^\dagger_{l\uparrow}, & \text{for } l \in B, \end{array} \tag{20.19}$$

we find

$$H(c, h) \to h(\hat{N} - L) + c\hat{N} + H(-c, h), \qquad \hat{N}_\uparrow \to L - \hat{N}_\uparrow, \quad \hat{N}_\downarrow \to \hat{N}_\downarrow. \tag{20.20}$$

This symmetry makes a link between the repulsive and attractive Hubbard models.

20.2 Nested Bethe ansatz

The Fock eigenstates of the Hubbard model with N electrons, M with spin down and $N-M$ with spin up, are expressible as follows

$$|N,M\rangle = \sum_{\{\sigma_j\}} \sum_{\{x_k\}} \psi_{\sigma_1 \ldots \sigma_N}(x_1,\ldots,x_N)\, c^\dagger_{x_1\sigma_1} \cdots c^\dagger_{x_N\sigma_N}|0\rangle, \tag{20.21}$$

where $\sum_{\{\sigma_j\}}$ denotes summation over all $N!/[M!(N-M)!]$ possible spin configurations. Due to the anticommutation relations between the Fermion operators, the amplitudes ψ are totally antisymmetric under simultaneous exchange of spin and space variables:

$$\psi_{\sigma_{Q1}\ldots\sigma_{QN}}(x_{Q1},\ldots,x_{QN}) = \mathrm{sign}(Q)\,\psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N), \tag{20.22}$$

where $Q=(Q1,Q2,\ldots,QN)$ is an element of the symmetric group S_N. The antisymmetry property (20.22) implies that the summation over spin configurations in (20.21) is redundant and we can set

$$|N,M\rangle = \frac{N!}{M!(N-M)!} \sum_{\{x_k\}} \psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N)\, c^\dagger_{x_1\sigma_1} \cdots c^\dagger_{x_N\sigma_N}|0\rangle, \tag{20.23}$$

where $(\sigma_1,\ldots,\sigma_N)$ is an arbitrary configuration of M electrons with spin down and $N-M$ electrons with spin up. Inserting (20.23) into the eigenvalue equation $H(c)|N,M\rangle = E(c)|N,M\rangle$, we obtain the "first quantized" version of the Schrödinger equation for the wavefunction ψ:

$$\begin{aligned} -\sum_{j=1}^{N}\sum_{\epsilon=\pm1} &\psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_j+\epsilon,\ldots,x_N) \\ &+2c\sum_{j<k}\delta(x_j,x_k)\,\psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N) \;=\; E(c)\psi_{\sigma_1\ldots\sigma_N}(x_1,\ldots,x_N). \end{aligned} \tag{20.24}$$

• $N=2$: In the case of two electrons, the Schrödinger equation (20.24) takes the form

$$\begin{aligned} -\psi_{\sigma_1\sigma_2}(x_1-1,x_2) &- \psi_{\sigma_1\sigma_2}(x_1+1,x_2) - \psi_{\sigma_1\sigma_2}(x_1,x_2-1) \\ &-\psi_{\sigma_1\sigma_2}(x_1,x_2+1) + 2c\delta(x_1,x_2)\,\psi_{\sigma_1\sigma_2}(x_1,x_2) = E\psi_{\sigma_1\sigma_2}(x_1,x_2). \end{aligned} \tag{20.25}$$

Let $Q=(Q1,Q2)\in S_2$ be a permutation of the labels of particle coordinates which defines the ordering sector $x_{Q1}\le x_{Q2}$ of mutual particle positions.

When $x_1<x_2$ or $x_1>x_2$, (20.25) reduces to the Schrödinger equation for free electrons on the chain and its solution is a superposition of plane waves. The nested Bethe ansatz form for the fermion wavefunction, see Eqs. (7.4)-(7.5), reads

$$\psi_{\sigma_1\sigma_2}(x_1,x_2) = \sum_{P\in S_2} \mathrm{sign}(QP) A_{\sigma_{Q1}\sigma_{Q2}}(k_{P1},k_{P2}) \exp\left(\mathrm{i}\sum_{\alpha=1}^{2} k_{P\alpha}x_{Q\alpha}\right), \tag{20.26}$$

where k_1 and k_2 are electron momenta. The substitution of this ansatz into Eq. (20.25) with $x_1\neq x_2$ leads to the total momentum K and energy E given by

$$K = k_1+k_2, \qquad E=-2(\cos k_1+\cos k_2). \tag{20.27}$$

When $x_1 = x_2$, the electrons occupy the same site and scatter with one another. The Bethe ansatz for the wavefunction (20.26) requires the scattering to be purely elastic, so that the momenta k_1 and k_2 are individually conserved (the electrons either keep or exchange their momenta). The scattering process is determined by two conditions. Firstly, we have to "match" the wavefunction defined in the two sectors $Q = (1,2)$ and $Q = (2,1)$ when $x_1 = x_2 = x$. This yields the conditions

$$A_{\sigma_1\sigma_2}(k_1,k_2) - A_{\sigma_1\sigma_2}(k_2,k_1) = A_{\sigma_2\sigma_1}(k_2,k_1) - A_{\sigma_2\sigma_1}(k_1,k_2). \tag{20.28}$$

Secondly, the Schrödinger equation (20.25) has to be fulfilled for $x_1 = x_2 = x$, which implies

$$\begin{aligned} &- \mathrm{e}^{-\mathrm{i}k_1} A_{\sigma_1\sigma_2}(k_1,k_2) + \mathrm{e}^{-\mathrm{i}k_2} A_{\sigma_1\sigma_2}(k_2,k_1) + \mathrm{e}^{\mathrm{i}k_2} A_{\sigma_2\sigma_1}(k_1,k_2) \\ &\quad -\mathrm{e}^{\mathrm{i}k_1} A_{\sigma_2\sigma_1}(k_2,k_1) - \mathrm{e}^{\mathrm{i}k_2} A_{\sigma_1\sigma_2}(k_1,k_2) + \mathrm{e}^{\mathrm{i}k_1} A_{\sigma_1\sigma_2}(k_2,k_1) \\ &\quad +\mathrm{e}^{-\mathrm{i}k_1} A_{\sigma_2\sigma_1}(k_1,k_2) - \mathrm{e}^{-\mathrm{i}k_2} A_{\sigma_2\sigma_1}(k_2,k_1) \\ &\quad +2[c + (\cos k_1 + \cos k_2)][A_{\sigma_1\sigma_2}(k_1,k_2) - A_{\sigma_1\sigma_2}(k_2,k_1)] \quad = \quad 0. \end{aligned} \tag{20.29}$$

With the aid of Eqs. (20.28) and (20.29) we can express any two of the four unknown A-amplitudes in terms of the other two. Simple algebra gives

$$A_{\sigma_2\sigma_1}(k_2,k_1) = \sum_{\sigma_1',\sigma_2'} S^{\sigma_1\sigma_2}_{\sigma_1'\sigma_2'}(k_1,k_2) A_{\sigma_1'\sigma_2'}(k_1,k_2), \tag{20.30}$$

where S is the two-particle scattering matrix with elements

$$S^{\sigma_1\sigma_2}_{\sigma_1'\sigma_2'}(k_1,k_2) = \frac{\sin k_1 - \sin k_2}{\sin k_1 - \sin k_2 + \mathrm{i}c} I^{\sigma_1\sigma_2}_{\sigma_1'\sigma_2'} + \frac{\mathrm{i}c}{\sin k_1 - \sin k_2 + \mathrm{i}c} \mathcal{P}^{\sigma_1\sigma_2}_{\sigma_1'\sigma_2'}. \tag{20.31}$$

Here, I and $\mathcal{P}$ are the identity and permutation operators, respectively. The natural parameterization of momenta k by rapidities λ is

$$\sin k = \lambda, \qquad k(\lambda) = \arcsin \lambda; \tag{20.32}$$

since the physical range of k is over a period 2π, $k(\lambda)$ is a two-sheeted function with branch points at $\lambda = \pm 1$. Within this parameterization, the S-matrix (20.31) can be expressed as

$$S_{12}(\lambda = \lambda_1 - \lambda_2) = \frac{\lambda}{\lambda + \mathrm{i}c} I + \frac{\mathrm{i}c}{\lambda + \mathrm{i}c} \mathcal{P}_{12}. \tag{20.33}$$

This matrix has the form of the S-matrix for the Heisenberg model (7.57) with the elements of the rational type

$$a(\lambda) = 1, \qquad b(\lambda) = \frac{\lambda}{\lambda + \mathrm{i}c}, \qquad c(\lambda) = \frac{\mathrm{i}c}{\lambda + \mathrm{i}c}, \qquad d(\lambda) = 0, \tag{20.34}$$

characteristic for the XXX Heisenberg chain.

We impose periodic boundary conditions on the wavefunction:

$$\begin{aligned} &\psi_{\sigma_1\sigma_2}(0,x_2) = \psi_{\sigma_1\sigma_2}(L,x_2), \qquad \psi_{\sigma_1\sigma_2}(x_1,0) = \psi_{\sigma_1\sigma_2}(x_1,L); \\ &\psi_{\sigma_1\sigma_2}(1,x_2) = \psi_{\sigma_1\sigma_2}(L+1,x_2), \quad \psi_{\sigma_1\sigma_2}(x_1,1) = \psi_{\sigma_1\sigma_2}(x_1,L+1). \end{aligned} \tag{20.35}$$

Inserting the Bethe ansatz (20.26) into these conditions yields

$$\exp(\mathrm{i}k_{P1}L)\, A_{\sigma_{Q2}\sigma_{Q1}}(k_{P2},k_{P1}) = A_{\sigma_{Q1}\sigma_{Q2}}(k_{P1},k_{P2}), \tag{20.36}$$

where the permutations $P, Q \in S_2$ are arbitrary. Choosing $Q = (2,1)$, one gets the eigenvalue problem

$$\begin{aligned}\exp(\mathrm{i}k_{P1}L)\, A_{\sigma_1\sigma_2}(k_{P2},k_{P1}) &= A_{\sigma_2\sigma_1}(k_{P1},k_{P2}) \\ &= \sum_{\sigma_1',\sigma_2'} S^{\sigma_1\sigma_2}_{\sigma_1'\sigma_2'}(k_{P2},k_{P1}) A_{\sigma_1'\sigma_2'}(k_{P2},k_{P1}).\end{aligned} \tag{20.37}$$

In the sector of both electrons with spin up, it follows from the explicit form of the S-matrix (20.31) that the boundary conditions corresponds to those of free fermions:

$$\exp(\mathrm{i}k_n L) = 1 \qquad n = 1,2. \tag{20.38}$$

Similarly as in the case of the Heisenberg chain, the wave numbers must be distinct, $k_1 \neq k_2$, in order to prevent the nullity of the wavefunction. The same result is obtained in the sector of both electrons with spin down.

In the sector of one electron with spin up and the other one with spin down, the diagonalized form of Eq. (20.37) has the form

$$\begin{aligned}&\left\{ \mathrm{e}^{\mathrm{i}k_{P1}L} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{\lambda_{P2}-\lambda_{P1}-\mathrm{i}c}{\lambda_{P2}-\lambda_{P1}+\mathrm{i}c} & 0 \\ 0 & 1 \end{pmatrix} \right\} \\ &\quad \times \begin{pmatrix} A_{\uparrow\downarrow}(k_{P2},k_{P1}) - A_{\downarrow\uparrow}(k_{P2},k_{P1}) \\ A_{\uparrow\downarrow}(k_{P2},k_{P1}) + A_{\downarrow\uparrow}(k_{P2},k_{P1}) \end{pmatrix} = 0.\end{aligned} \tag{20.39}$$

This eigenvalue equation has two possible solutions. The first solution, corresponding to the coefficients $A_{\uparrow\downarrow}(k_{P2},k_{P1}) = -A_{\downarrow\uparrow}(k_{P2},k_{P1})$, reads

$$\exp(\mathrm{i}k_{P1}L) = \frac{\lambda_{P1}-\lambda_{P2}+\mathrm{i}c}{\lambda_{P1}-\lambda_{P2}-\mathrm{i}c}. \tag{20.40}$$

Introducing $\Lambda_1 = (\sin k_1 + \sin k_2)/2$, Eq. (20.40) can be re-expressed in a more symmetric way

$$\exp[\mathrm{i}k(\lambda_n)L] = \frac{\lambda_n - \Lambda_1 + \mathrm{i}c'}{\lambda_n - \Lambda_1 - \mathrm{i}c'} \qquad n = 1,2, \tag{20.41}$$

where $c' = c/2$. It follows from (20.40) that $\exp(\mathrm{i}k_1 L)\exp(\mathrm{i}k_2 L) = 1$. Thus Λ_1 is determined by the condition

$$\prod_{n=1}^{2} \frac{\Lambda_1 - \lambda_n + \mathrm{i}c'}{\Lambda_1 - \lambda_n - \mathrm{i}c'} = 1. \tag{20.42}$$

The second solution to (20.39), which corresponds to $A_{\uparrow\downarrow}(k_{P2},k_{P1}) = A_{\downarrow\uparrow}(k_{P2},k_{P1}) = A_{\uparrow\downarrow}(k_{P1},k_{P2})$, is equivalent to the previous one (20.38).

• Arbitrary N: The generalization of the above scheme to N electrons is straightforward. The Bethe ansatz for the solution ψ of the Schrödinger equation in the ordering sector Q with $x_{Q1} \leq x_{Q2} \leq \ldots \leq x_{QN}$ is

$$\begin{aligned}\psi_{\sigma_1\sigma_2\ldots\sigma_N}(x_1, x_2, \ldots, x_N) &= \sum_{P\in S_N} \mathrm{sign}(QP) A_{\sigma_{Q1}\sigma_{Q2}\ldots\sigma_{QN}}(k_{P1}, k_{P2}, \ldots, k_{PN}) \\ &\quad \times \exp\left(\mathrm{i}\sum_{\alpha=1}^{N} k_{P\alpha} x_{Q\alpha}\right). \end{aligned} \tag{20.43}$$

Substituting this ansatz into the Schrödinger equation (20.24) for the case $x_n \neq x_m$ $(n, m = 1, \ldots, N; n \neq m)$, the total momentum and energy of the Hamiltonian $H(c)$ is obtained in the usual form

$$K = \sum_{n=1}^{N} k_n, \qquad E = -2\sum_{n=1}^{N} \cos k_n. \tag{20.44}$$

The Bethe ansatz wavefunction (20.43) is by construction antisymmetric under simultaneous exchange of spin and space variables. This fact assures the Schrödinger equation (20.24) to be satisfied when three or more electrons are occupying the same site. The only non-trivial case to consider is the presence of two electrons on the same site. Using the single valuedness of the wavefunction and solving the matching conditions at the Q-sector boundaries, one gets the nearest-neighbour electron scattering between the amplitudes

$$A_{\ldots\sigma_j\sigma_i\ldots}(\ldots k_v, k_u \ldots) = \sum_{\sigma_i'\sigma_j'} S^{\sigma_i\sigma_j}_{\sigma_i'\sigma_j'}(k_u, k_v) A_{\ldots\sigma_i'\sigma_j'\ldots}(\ldots k_u, k_v \ldots), \tag{20.45}$$

where the two-particle S-matrix is given by (20.31).

We impose periodic boundary conditions on the wavefunction:

$$\begin{aligned}\psi_{\sigma_1\ldots\sigma_N}(x_1, \ldots, \underbrace{0}_{n}, \ldots, x_N) &= \psi_{\sigma_1\ldots\sigma_N}(x_1, \ldots, \underbrace{L}_{n}, \ldots, x_N), \\ \psi_{\sigma_1\ldots\sigma_N}(x_1, \ldots, \underbrace{1}_{n}, \ldots, x_N) &= \psi_{\sigma_1\ldots\sigma_N}(x_1, \ldots, \underbrace{L+1}_{n}, \ldots, x_N),\end{aligned} \tag{20.46}$$

where the underbraced particle position $n = 1, \ldots, N$. Inserting the Bethe ansatz (20.43) into these conditions yields

$$\begin{aligned}A_{\sigma_{Q2}\ldots\sigma_{QN}\sigma_{Q1}}(k_{P2}, \ldots, k_{PN}, k_{P1}) &= \exp(-\mathrm{i}k_{P1}L) \\ &\quad \times A_{\sigma_{Q1}\sigma_{Q2}\ldots\sigma_{QN}}(k_{P1}, k_{P2}, \ldots, k_{PN}).\end{aligned} \tag{20.47}$$

These equations coincide with the fermion boundary conditions (9.10) in the generalized Bethe ansatz, while the scattering formula (20.45) is identical to (9.12). We can therefore apply the QISM procedure explained in Sect. 9, working with the weights a, b, c and d defined in (20.34). In the sector with $N_\downarrow = M$ $(M \leq N/2)$ spin-down electrons and $N_\uparrow = N - M$ spin-up electrons, we introduce M auxiliary spectral parameters $\Lambda_1, \ldots, \Lambda_M$. Using the shift $\Lambda_\alpha \to \Lambda_\alpha - \mathrm{i}c'$ in the set of equations (9.35), these parameters are determined by

$$\prod_{n=1}^{N} \frac{\Lambda_\alpha - \lambda_n + \mathrm{i}c'}{\Lambda_\alpha - \lambda_n - \mathrm{i}c'} = \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}c}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}c}, \qquad \alpha = 1, \ldots, M. \tag{20.48}$$

The quantization condition for momenta (9.37) now becomes

$$\exp[\mathrm{i}k(\lambda_n)L] = \prod_{\alpha=1}^{M} \frac{\lambda_n - \Lambda_\alpha + \mathrm{i}c'}{\lambda_n - \Lambda_\alpha - \mathrm{i}c'}, \qquad n = 1, \ldots, N. \tag{20.49}$$

Since the dispersion relations for small λ are

$$k(\lambda) = \arcsin\lambda \sim \lambda, \qquad e(\lambda) = -2\sqrt{1-\lambda^2} \sim -2 + \lambda^2, \tag{20.50}$$

the low density limit of the Hubbard model is equivalent to the problem of spin-$\frac{1}{2}$ fermions with δ-function interactions, see Eqs. (10.27) and (10.28).

20.3 Ground-state properties of the repulsive Hubbard model

In the ground state of the repulsive regime $c > 0$, all roots k_n (or λ_n) and Λ_α of the Bethe equations (20.48) and (20.49) are real. Since $k(\lambda)$ is a two-sheeted function, we shall keep in the formalism the k-variable rather than the spectral parameter $\lambda = \sin k$. Taking the logarithm of the Bethe equations we arrive at

$$k_n L = 2\pi I_n - \sum_{\alpha=1}^{M} \theta\left(2(\sin k_n - \Lambda_\alpha)\right), \quad n = 1, \ldots, N; \tag{20.51}$$

$$\sum_{n=1}^{N} \theta\left(2(\Lambda_\alpha - \sin k_n)\right) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \theta(\Lambda_\alpha - \Lambda_\beta), \quad \alpha = 1, \ldots, M, \tag{20.52}$$

where I_n, J_α are integers or half-integers and $\theta(x) = 2\arctan(x/c)$. Quantum numbers I_n and J_α are densely packed around 0 in the ground state, hence the total momentum $K_0 = (2\pi/L)(\sum_n I_n + \sum_\alpha J_\alpha) = 0$. The roots $\{k_n\}$ are known as charge momenta and $\{\Lambda_\alpha\}$ as spin rapidities.

20.3.1 Fredholm integral equations for distribution functions

We consider the thermodynamic limit $L, N, M \to \infty$, with the fixed particle densities $n = N/L$ and $n_\downarrow = M/L$. The continuous k's and Λ's are distributed symmetrically around zero, with the densities $\rho(k) = \rho(-k)$ and $\sigma(\Lambda) = \sigma(-\Lambda)$ between some limits $\pm q$ and $\pm Q$, respectively. The normalizations

$$n = n_\uparrow + n_\downarrow = \int_{-q}^{q} \mathrm{d}k\, \rho(k), \qquad n_\downarrow = \int_{-Q}^{Q} \mathrm{d}\Lambda\, \sigma(\Lambda) \tag{20.53}$$

imply implicit relationships between the densities of up-spin and down-spin electrons and the integration limits, Integral equations satisfied by the distribution functions are obtained by making the continualization of (20.51) and (20.52) and consequently by taking the derivatives of the continuum equations with respect to k and Λ:

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_{-Q}^{Q} \mathrm{d}\Lambda\, a_1(\sin k - \Lambda)\sigma(\Lambda), \tag{20.54}$$

$$\sigma(\Lambda) = \int_{-q}^{q} \mathrm{d}k\, a_1(\Lambda - \sin k)\rho(k) - \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma(\Lambda'), \tag{20.55}$$

where $a_n(x) = \pi^{-1}(nc')/[x^2 + (nc')^2]$. These equations determine the distribution functions also beyond their limits, i.e. $\rho(k)$ for $|k| > q$ and $\sigma(\Lambda)$ for $|\Lambda| > Q$. In such cases, $\rho(k)$ and $\sigma(\Lambda)$ represent the hole distributions at $T = 0$.

It is convenient to pass from the above canonical ensemble to the grand-canonical one, with the magnetic field h and the chemical potential μ of particles as the control variables. The ground-state energy per site of the Hamiltonian (20.16) is expressible as

$$e_0 \equiv \frac{E_0}{L} = \int_{-q}^{q} \mathrm{d}k\,(-2\cos k - h)\rho(k) + 2h\int_{-Q}^{Q} \mathrm{d}\Lambda\,\sigma(\Lambda). \tag{20.56}$$

Let us introduce a coupled pair of dressed energies $\epsilon(k) = \epsilon(-k)$ and $\epsilon_1(\Lambda) = \epsilon_1(-\Lambda)$ which satisfy the integral equations

$$\epsilon(k) = -2\cos k - \mu - h + \int_{-Q}^{Q} \mathrm{d}\Lambda\, a_1(\sin k - \Lambda)\epsilon_1(\Lambda), \tag{20.57}$$

$$\epsilon_1(\Lambda) = 2h + \int_{-q}^{q} \mathrm{d}k\, a_1(\Lambda - \sin k)\cos k\,\epsilon(k) - \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\epsilon_1(\Lambda'). \tag{20.58}$$

The integration limits $\pm q$ and $\pm Q$ are the points at which the dressed energies change sign; these conditions determine the limits q and Q as functions of the magnetic field h and the chemical potential μ. In particular,

$$\epsilon(\pm q) = 0, \qquad \epsilon(k)\begin{cases} < 0 & \text{for } |k| < q, \\ > 0 & \text{for } |k| > q \end{cases} \tag{20.59}$$

and, similarly,

$$\epsilon_1(\pm Q) = 0, \qquad \epsilon_1(\Lambda)\begin{cases} < 0 & \text{for } |\Lambda| < Q, \\ > 0 & \text{for } |\Lambda| > Q. \end{cases} \tag{20.60}$$

To document that our μ is consistent with the general definition of the chemical potential, we first add to and subtract from Eq. (20.56) the term $\mu\int_{-q}^{q}\mathrm{d}k\,\rho(k)$, then express $(-2\cos k - \mu - h)$ by using Eq. (20.57) and finally express $\rho(\lambda)$ in the integral $\int_{-q}^{q}\mathrm{d}k\,\epsilon(k)\rho(k)$ by using Eq. (20.54), to obtain

$$\begin{aligned} E_0 = {} & \frac{1}{2\pi}\int_{-q}^{q}\mathrm{d}k\,\epsilon(k)L + \mu N + \Bigg\{2h\int_{-Q}^{Q}\mathrm{d}\Lambda\,\sigma(\Lambda) \\ & + \int_{-q}^{q}\mathrm{d}k\int_{-Q}^{Q}\mathrm{d}\Lambda\, a_1(\sin k - \Lambda)\cos k\,[\epsilon(k)\sigma(\Lambda) - \rho(k)\epsilon_1(\Lambda)]\Bigg\}. \end{aligned} \tag{20.61}$$

It can be readily shown that the expression between curled brackets vanishes. With regard to the Gibbs relation $E_0 = -PL + \mu N$, the pressure is given by

$$P = -\frac{1}{2\pi}\int_{-q}^{q}\mathrm{d}k\,\epsilon(k) \tag{20.62}$$

and the parameter μ is indeed the chemical potential.

Using the response of the ground state to a perturbation it can be shown that $\epsilon(k)$ and $\epsilon_1(\Lambda)$ are related to elementary low-lying excitations. In the case of charge (spinless) excitations of particle type, we take a particle from q to $k_p > q$, or alternatively from $-q$ to $k_p < -q$. This excited state has the energy change and the momentum given by

$$\Delta E(k_p) = \epsilon(k_p), \qquad K(k_p) = 2\pi \int_q^{k_p} \mathrm{d}k\, \rho(k). \tag{20.63}$$

Charge excitations of hole type correspond to taking a particle from $0 < k_h < q$ to $q + 2\pi/L$, or alternatively from $-q < k_h < 0$ to $-q - 2\pi/L$. This state is characterized by

$$\Delta E(k_h) = -\epsilon(k_h), \qquad K(k_h) = 2\pi \int_{k_h}^{q} \mathrm{d}k\, \rho(k). \tag{20.64}$$

Similarly, we can generate spin excitations by taking a particle from $\pm Q$ to $|\Lambda_p| > Q$ or creating a hole at $|\Lambda_h| < Q$. The corresponding excited states are characterized by

$$\Delta E(\Lambda_p) = \epsilon_1(\Lambda_p), \qquad K(\Lambda_p) = 2\pi \int_Q^{\Lambda_p} \mathrm{d}\Lambda\, \sigma(\Lambda); \tag{20.65}$$

$$\Delta E(\Lambda_h) = -\epsilon_1(\Lambda_h), \qquad K(\Lambda_h) = 2\pi \int_{\Lambda_h}^{Q} \mathrm{d}\Lambda\, \sigma(\Lambda). \tag{20.66}$$

20.3.2 Ground-state phase diagram

Different phases at zero temperature are most easily identified via the integration limits q and Q in the integral equations (20.54), (20.55) and (20.57), (20.58). The physical range of q is $[0, \pi]$ and that of Q is $[0, \infty]$. Before establishing the classification of phases, we discuss some values of the limits q and/or Q which are of special interest.

The case $q = 0$ automatically implies $Q = 0$ and we have an empty system $(n = 0)$. The opposite case $q = \pi$ (Q is arbitrary) implies that the band is half filled, i.e. there is one electron per site $(n = 1)$. This can be seen by applying $\int_{-\pi}^{\pi} \mathrm{d}k$ to both sides of Eq. (20.54), defining the function $f_\Lambda(x) = a_1(x - \Lambda) + a_1(x + \Lambda)$ which possess the symmetry $f_\Lambda(x) = f_\Lambda(-x)$ and finally using the identities

$$\int_{-\pi}^{\pi} \mathrm{d}k\, \cos k\, f_\Lambda(\sin k) = 2 \int_0^{\pi} \mathrm{d}k\, \cos k\, f_\Lambda(\sin k) = 0. \tag{20.67}$$

Here, the second equality can be proved via the substitution $k = \pi - k'$.

For $Q = 0$ (q is arbitrary), the ground state is completely magnetized $(n_\uparrow = n, n_\downarrow = 0)$. In the limiting case $Q \to \infty$, applying $\int_{-\infty}^{\infty} \mathrm{d}\Lambda$ to Eq. (20.55) and using that $\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, a_n(\Lambda) = 1$, we obtain

$$n_\downarrow = \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda) = \frac{1}{2} \int_{-q}^{q} \mathrm{d}k\, \rho(k) = \frac{n}{2}, \tag{20.68}$$

i.e. the magnetization is zero or, equivalently, $h = 0$.

Based on this brief analysis, we recognize five distinct phases in the (μ, h) plane.

- Phase I: $q = 0$, $Q = 0$; empty band.

  This phase corresponds to an empty lattice $n_\uparrow = n_\downarrow = 0$. The dressed energies in (20.57) and (20.58) must be positive, which implies that

$$h \leq -2 - \mu \qquad (\mu < -2). \tag{20.69}$$

- Phase II: $0 < q < \pi$, $Q = 0$; partially filled, spin polarized band.

  This region of parameters corresponds to the particle densities between the empty lattice and the half-filled band, $0 < n < 1$, with completely polarized spins, $n_\uparrow = n$ and $n_\downarrow = 0$. The integral equations for the dressed energies simplify to

$$\epsilon(k) = -2\cos k - \mu - h, \qquad \epsilon(\pm q) = 0, \tag{20.70}$$

$$\epsilon_1(\Lambda) = 2h + \int_{-q}^{q} \mathrm{d}k\, a_1(\Lambda - \sin k)\cos k\, \epsilon(k) \geq 0. \tag{20.71}$$

  The requirement $\epsilon(\pm q) = 0$ implies the relation

$$\cos q = -\frac{1}{2}(\mu + h). \tag{20.72}$$

  Since $-1 < \cos q < 1$, we have the following conditions

$$h \geq -2 - \mu \qquad (\mu < -2), \qquad h \leq 2 - \mu. \tag{20.73}$$

  The positiveness of $\epsilon_1(\Lambda)$ implies that

$$h \geq h_c(q) = \frac{c}{\pi}\int_0^q \mathrm{d}k\, \cos k\, \frac{\cos k - \cos q}{(c')^2 + \sin^2 k}. \tag{20.74}$$

  According to (20.54), the distribution of k roots is constant, $\rho(k) = 1/(2\pi)$, so $q = \pi n$. In the limit $c \to \infty$, we can express the critical field value of the field $h_c(q)$ as a function of the particle density as follows

$$h_c(q) = \frac{2}{c}\left[n - \frac{\sin(2\pi n)}{2\pi}\right] + O(1/c^3). \tag{20.75}$$

- Phase III: $q = \pi$, $Q = 0$; half filled, spin polarized band.

  For this case, we have the half-filled band $n = 1$ with completely polarized spins, $n_\uparrow = n = 1$ and $n_\downarrow = 0$. The integral equations for the dressed energies are solved explicitly:

$$\epsilon(k) = -2\cos k - \mu - h, \tag{20.76}$$

$$\epsilon_1(\Lambda) = 2h - 4\Re e\sqrt{1 - (\Lambda - \mathrm{i}c')^2} + 2c. \tag{20.77}$$

Here, we used the formula

$$\int_{-\pi}^{\pi} \mathrm{d}k\, 2\cos^2 k\, \frac{1}{\pi}\frac{c'}{(c')^2+(\sin k-\Lambda)^2} = 4\Re e\sqrt{1-(\Lambda-\mathrm{i}c')^2}-2c. \tag{20.78}$$

The energy signs $\epsilon(k)\le 0$ and $\epsilon_1(\Lambda)\ge 0$ lead to the conditions

$$h\ge 2-\mu, \qquad h\ge h_c = 2\sqrt{1+(c')^2}-c, \tag{20.79}$$

where h_c is the critical field (20.74) taken at $q=\pi$, $h_c\equiv h_c(\pi)$.

- Phase IV: $0<q<\pi$, $0<Q\le\infty$; partially filled and magnetized band.

  This region corresponds to $0<n<1$ and $0<n_\downarrow\le n/2$. The analytic results can be obtained only for $h=0$ ($n_\downarrow=n_\uparrow=n/2$), in the limit of small densities $n\approx 0$ and close to half-filling $n\approx 1$.

- Phase V: $q=\pi$, $0<Q\le\infty$; half filled, partially magnetized band.

  This phase corresponds to $n=1$ and $0<n_\downarrow\le 1/2$. The integral equations for the dressed energies become

$$\epsilon(k) = -2\cos k-\mu-h+\int_{-Q}^{Q}\mathrm{d}\Lambda\, a_1(\sin k-\Lambda)\epsilon_1(\Lambda), \tag{20.80}$$

$$\epsilon_1(\Lambda) = 2h-4\Re e\sqrt{1-(\Lambda-\mathrm{i}c')^2}+2c - \int_{-Q}^{Q}\mathrm{d}\Lambda'\, a_2(\Lambda-\Lambda')\epsilon_1(\Lambda'). \tag{20.81}$$

The inequality $\epsilon(k)\le 0$ applies to all $k\in[-\pi,\pi]$. In the interior of Phase V, $\epsilon(k)$ is strictly negative for all values of k, including $\epsilon(\pm\pi)<0$. The equality $\epsilon(\pm\pi)=0$ determines the boundary between Phases IV and V. It is important to note that the particle density $n=1$ in the whole region V. Therefore, for a fixed value of h, increasing μ by a small amount does not change n. This is an evidence that all eigenenergies of the Hubbard Hamiltonian with one additional particle are separated from the ground-state energy by a finite gap. This unconventional state of the electron system, driven entirely by electron-electron interactions, is known as a Mott insulator [2]. The proof that the half filled Hubbard model is an insulator is usually based on the discontinuity of the chemical potentials

$$\begin{aligned}\mu_-(c,h) &= E_0(L;c,h)-E_0(L-1;c,h),\\ \mu_+(c,h) &= E_0(L+1;c,h)-E_0(L;c,h),\end{aligned} \tag{20.82}$$

where $E_0(N;c,h)$ is the ground-state energy of N electrons on the chain of L sites. The chemical potential $\mu_-(c,h)$ is related to the half filled ground state. Having the explicit form of $\epsilon(k)$, it is determined by the boundary condition $\epsilon(\pm\pi)=0$ between Phases IV and V; for $h=0$, this will be done in the next Sec. 20.3.3. The chemical potential $\mu_+(c,h)$ is the energy necessary to add one extra electron into the half filled ground state. For $h=0$,

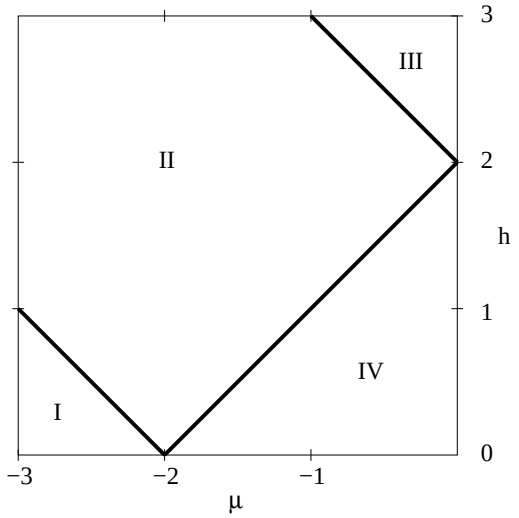


Fig. 20.1. Ground-state phase diagram for non-interacting electrons as a function of chemical potential μ and magnetic field $h > 0$.

the symmetry relation (20.18) implies $E_0(2L - N; c, 0) = 2c(L - N) + E_0(N; c, 0)$. Choosing $N = L - 1$ we arrive at $\mu_+(c, 0) + \mu_-(c, 0) = 2c$, i.e. the gap is determined by

$$\text{gap} \equiv \mu_+(c, 0) - \mu_-(c, 0) = 2c - 2\mu_-(c, 0). \tag{20.83}$$

The ground state phase diagram in the (μ, h) plane is pictured in Fig. 20.1 for non-interacting electrons ($c = 0$, the system is conducting and the insulator Phase V is absent) and in Fig. 20.2 for interacting electrons ($c = 2$).

20.3.3 Analytic results for zero field and half filled band

The absolute ground state corresponds to the zero field $h = 0$ ($Q \to \infty$) and the half-filled band $n = 1$ ($q = \pi$). In this case, the integral equations for the distribution functions and the dressed energies can be solved by Fourier series techniques.

Let us first consider the case $h = 0$ ($Q \to \infty$), the electron density n is not fixed. From Eq. (20.55) we obtain

$$\begin{aligned} \hat{\sigma}(\omega) &= \int_{-\infty}^{\infty} \mathrm{d}\Lambda \, \exp(-\mathrm{i}\omega\Lambda)\sigma(\Lambda) \\ &= \int_{-q}^{q} \mathrm{d}k \, \rho(k) \exp\left(-\mathrm{i}\omega \sin k - c'|\omega|\right) - \hat{\sigma}(\omega) \exp(-c|\omega|), \end{aligned} \tag{20.84}$$

where we used that the Fourier transform of $a_n(x)$ is $\hat{a}_n(\omega) = \exp(-nc'|\omega|)$. Expressing explicitly $\hat{\sigma}(\omega)$ and Fourier transforming back we find

$$\sigma(\Lambda) = \int_{-q}^{q} \mathrm{d}k \, \frac{1}{2c} \frac{1}{\cosh \frac{\pi}{c}(\Lambda - \sin k)} \rho(k). \tag{20.85}$$

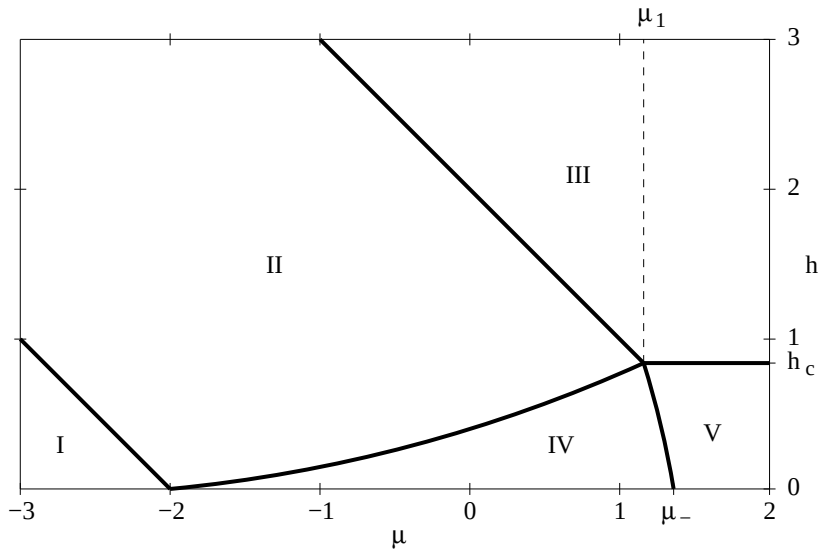


Fig. 20.2. Ground-state phase diagram for interacting $(c = 2)$ Hubbard electrons as a function of chemical potential μ and magnetic field $h > 0$. The critical field h_c is given by (20.79), $\mu_1 = 2 - h_c$ and μ_- is given by (20.95).

Inserting this relation into the rhs of Eq. (20.54) for $\rho(k)$ results in the integral equation

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_{-q}^{q} \mathrm{d}k'\, R(\sin k - \sin k')\rho(k'), \tag{20.86}$$

where

$$R(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\exp(-\mathrm{i}\omega x)}{1 + \exp(c|\omega|)}. \tag{20.87}$$

The integral equations for the dressed energies (20.57) and (20.58) can be solved in an analogous way, with the final result

$$\epsilon_1(\Lambda) = \int_{-q}^{q} \mathrm{d}k\, \frac{1}{2c} \frac{\cos k}{\cosh \frac{\pi}{c}(\Lambda - \sin k)} \epsilon(k), \tag{20.88}$$

$$\epsilon(k) = -2\cos k - \mu + \int_{-q}^{q} \mathrm{d}k'\, \cos k'\, R(\sin k - \sin k')\epsilon(k'). \tag{20.89}$$

If moreover the band is half filled $(q = \pi)$, the application of the Fourier method for periodic functions leads to the root densities

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{J_0(\omega)\cos(\omega \sin k)}{1 + \exp(c|\omega|)} \equiv \rho_0(k), \tag{20.90}$$

$$\sigma(\Lambda) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{J_0(\omega)}{2\cosh(c'|\omega|)} \exp(-\mathrm{i}\omega\Lambda) \equiv \sigma_0(\Lambda), \tag{20.91}$$

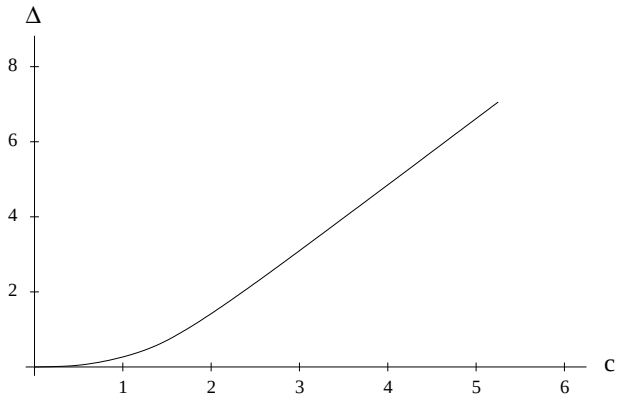


Fig. 20.3. Charge gap Δ at half filling versus the coupling strength c of electrons.

where J_0 is the Bessel function. The ground state energy per site (20.56) is obtained in the form

$$e_0 = -4 \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_0(\omega) J_1(\omega)}{1 + \exp(c\omega)}. \tag{20.92}$$

The dressed energies are obtained in a similar way and read

$$\epsilon(k) = -2\cos k - \mu - 4 \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega) \cos(\omega \sin k)}{1 + \exp(c\omega)}, \tag{20.93}$$

$$\epsilon_1(\Lambda) = -2 \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega) \cos(\Lambda\omega)}{\cosh(c'\omega)}. \tag{20.94}$$

The boundary condition between Phases IV and V $\epsilon(\pm\pi) = 0$ determines

$$\mu_-(c, 0) = 2 - 4 \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)}{1 + \exp(c\omega)}. \tag{20.95}$$

Inserting this solution into (20.83), the gap for the repulsive Hubbard model at half filling is given by

$$\mathrm{gap} = -4 + 2c + 8 \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)}{1 + \exp(c\omega)}. \tag{20.96}$$

The dependence of the charge gap on the coupling c is pictured in Fig. 20.3. It is seen that the Mott transition from conductor to insulator occurs at the trivial critical value $c_c = 0$.

As the values of the integration limits $q = \pi$ and $Q \to \infty$ are on the border of their physical values, low-lying excitations are only of hole type, see Eqs. (20.64) and (20.66). Charge (spinless) hole excitations, called holons or antiholons, are gaped. Spin (charge neutral) hole excitations, called spinons, are gapless.

20.3.4 Expansions around special points

• **Zero field, almost half filled band:** When the magnetic field $h = 0$ and the electron density n is slightly below 1, the integral equations for the root density $\rho(k)$ and the dressed energy $\epsilon(k)$ can be solved by using an iterative procedure [6]; in what follows, we shall study only $\rho(k)$. For $h = 0$, Eq. (20.86) implies that $\rho(k)$ exhibits, besides the reflection symmetry $\rho(k) = \rho(-k)$, also the following symmetry

$$\rho(\pi - k) = -\rho(k) + \frac{1}{\pi}. \tag{20.97}$$

For q slightly smaller than π, the integral in (20.86) can be re-expressed as follows

$$\begin{aligned}\int_{-q}^{q} \mathrm{d}k'\, R(\sin k - \sin k')\rho(k') \;&=\; \int_{0}^{q} \mathrm{d}k'\, \mathbf{R}(k,k')\rho(k') = \int_{0}^{\pi} \mathrm{d}k'\, \mathbf{R}(k,k')\rho(k') \\ &\quad - \int_{0}^{\pi-q} \mathrm{d}k'\, \mathbf{R}(k,k')\rho(\pi - k'),\end{aligned} \tag{20.98}$$

where $\mathbf{R}(k,k') = R(\sin k - \sin k') + R(\sin k + \sin k')$. The symmetry (20.97) implies that $\int_0^\pi \mathrm{d}k'\, \mathbf{R}(k,k')\rho(k') = \int_0^\pi \mathrm{d}k'\, \mathbf{R}(k,k')/(2\pi)$. Thus we rewrite Eq. (20.86) as

$$\rho(k) = \rho_0(k) - \cos k \int_{0}^{\pi-q} \mathrm{d}k'\, \mathbf{R}(k,k')\rho(\pi - k'), \tag{20.99}$$

where $\rho_0(k)$ is the root density at half filling, see Eq. (20.90). This equation can be treated iteratively and the functions under consideration can be expanded in powers of small difference $\pi - q$. However we prefer to use as the smallness parameter the deviation of the electron density from one

$$\delta \equiv 1 - n = 1 - \int_{-q}^{q} \mathrm{d}k\, \rho(k) = 2\int_{0}^{\pi-q} \mathrm{d}k\, \rho(\pi - k). \tag{20.100}$$

Considering the expansions

$$\pi - q = \sum_{n=1}^{\infty} a_n \delta^n, \qquad \rho(k) = \sum_{n=0}^{\infty} \rho_n(k)\delta^n \tag{20.101}$$

in Eq. (20.99) and taking in the integration Taylor expansions around $k' = 0$, we obtain the first few terms in the form

$$\begin{array}{ll} a_1 = [2\rho_0(\pi)]^{-1}, & \rho_1(k) = -\cos kR(\sin k), \\ a_2 = -2R(0)a_1^2, & \rho_2(k) = 0, \\ a_3 = 4a_1^3R^2(0) - a_1^4\rho_0''(\pi)/3, & \rho_3(k) = -a_1^2 \cos kR''(\sin k)/6. \end{array} \tag{20.102}$$

The ground state energy per site is then given by

$$e_0(n) = -2\int_{-q}^{q} \mathrm{d}k\, \cos k = e_0(1) - \mu_-(c,0)\delta + \frac{a_1^2\alpha_1}{3}\delta^3 + O(\delta^4), \tag{20.103}$$

where $\mu_-(c,0)$ is the $h=0$ chemical potential at the transition to half-filling given by (20.95) and

$$\alpha_1 = 1 - 2\int_0^\infty \mathrm{d}\omega\, \frac{\omega J_1(\omega)}{1+\exp(c\omega)}. \tag{20.104}$$

The chemical potential as a function of the density is given by

$$\mu = \frac{\partial e_0(n)}{\partial n} = \mu_-(c,0) - a_1^2\alpha_1\delta^2 + O(\delta^3). \tag{20.105}$$

The inversion of this relation implies

$$n(\mu) \sim 1 - \frac{1}{a_1\sqrt{\alpha_1}}\sqrt{\mu_-(c,0)-\mu}. \tag{20.106}$$

• **Zero field, low density:** For small densities $n \ll 1$, or equivalently small $q \ll \pi$, the integral equation for $\rho(k)$ (20.86) becomes

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_0^q \mathrm{d}k'\, \mathbf{R}(k,k')\rho(k'). \tag{20.107}$$

This equation can be treated iteratively in close analogy with Eq. (20.99). Using the expansions

$$q = \sum_{j=1}^\infty \tilde{a}_j n^j, \qquad \rho(k) = \frac{1}{2\pi} + \sum_{j=1}^\infty \tilde{\rho}_j(k) n^j, \tag{20.108}$$

we have

$$\begin{array}{ll} \tilde{a}_1 = \pi, & \tilde{\rho}_1(k) = \cos k R(\sin k), \\ \tilde{a}_2 = -2\pi^2 R(0), & \tilde{\rho}_2(k) = 0, \\ \tilde{a}_3 = 4\pi^3 R^2(0), & \tilde{\rho}_3(k) = \pi^2 \cos k R''(\sin k)/6. \end{array} \tag{20.109}$$

Note that these coefficients can be obtained from the ones in (20.102) by setting $\rho_0(k) = 1/(2\pi)$ and then assuming that $\tilde{\rho}_j(k) = \rho_j(\pi - k)$. The ground state energy per site is given by

$$e_0(n) = -2\int_{-q}^q \mathrm{d}k\, \cos k = -2n + \frac{\pi^2}{3}n^3 + O(n^4). \tag{20.110}$$

The dependence of the chemical potential on the density follows from

$$\mu = \frac{\partial e_0(n)}{\partial n} = -2 + \pi^2 n^2 + O(n^3). \tag{20.111}$$

Inverting this relation we arrive at

$$n(\mu) \sim \frac{1}{\pi}\sqrt{2+\mu}. \tag{20.112}$$

• **Half filled band, non-zero field:** Now we consider the half filled case $n=1$ ($q=\pi$) in the coupled integral equations (20.54) and (20.55). Using that $\int_{-\pi}^{\pi} \mathrm{d}k\, a_1^2(\Lambda - \sin k)\cos k = 0$, the equation for $\sigma(\Lambda)$ reads

$$\sigma(\Lambda) + \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma(\Lambda') = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} a_1(\Lambda - \sin k). \tag{20.113}$$

The ground-state energy per site (20.56) is written as follows

$$e_0 = -h + \int_{-Q}^{Q} \mathrm{d}\Lambda\, \sigma(\Lambda) \left[2h - 2 \int_{-\pi}^{\pi} \mathrm{d}k\, a_1(\Lambda - \sin k) \cos^2 k \right]. \tag{20.114}$$

To establish the relationship between the magnetic field h and the integration limit Q of Λ's, we change infinitesimally $Q \to Q + \Delta Q$. The energy change is given by

$$\begin{aligned} \Delta e_0 &= 2\Delta Q \sigma(Q) \left[2h - 2 \int_{-\pi}^{\pi} \mathrm{d}k\, a_1(Q - \sin k) \cos^2 k \right] \\ &\quad + \int_{-Q}^{Q} \mathrm{d}\Lambda\, \Delta\sigma(\Lambda) \left[2h - 2 \int_{-\pi}^{\pi} \mathrm{d}k\, a_1(\Lambda - \sin k) \cos^2 k \right]. \end{aligned} \tag{20.115}$$

Here, the distribution change $\Delta\sigma(\Lambda)$ satisfies the differential equation

$$\Delta\sigma(\Lambda) + \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda') \Delta\sigma(\Lambda') = -\Delta Q \sigma(Q) \left[a_2(\Lambda - Q) + a_2(\Lambda + Q) \right]. \tag{20.116}$$

Proceeding analogously as in Sect. 14.2, we find that

$$\frac{\Delta e_0}{4\sigma(Q)\Delta Q} = -2\pi P(Q) + hL(Q), \tag{20.117}$$

where the functions $L(\Lambda)$ and $P(\Lambda)$ satisfy the integral equations

$$L(\Lambda) + \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda') L(\Lambda') = 1, \tag{20.118}$$

$$P(\Lambda) + \int_{-Q}^{Q} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda') P(\Lambda') = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} a_1(\Lambda - \sin k) \cos^2 k. \tag{20.119}$$

The extremal conditions for the energy minimum $\Delta e_0 / \Delta Q = 0$ implies that for a given Q the magnetic field is

$$h = \frac{2\pi P(Q)}{L(Q)}. \tag{20.120}$$

The magnetization per site is given by

$$\lim_{L\to\infty} \frac{1}{L} \langle S^z_{\mathrm{tot}} \rangle \equiv \frac{s}{2}, \qquad s = n_\uparrow - n_\downarrow = 1 - 2 \int_{-Q}^{Q} \mathrm{d}\Lambda\, \sigma(\Lambda). \tag{20.121}$$

Integrating Eq. (20.113) over $\Lambda \in [-\infty, \infty]$ and using that $\hat{a}_1(0) = \hat{a}_2(0) = 1$, we obtain the exact relation

$$\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda) + \int_{-Q}^{Q} \mathrm{d}\Lambda\, \sigma(\Lambda) = 1. \tag{20.122}$$

Consequently, another representation of s, alternative to (20.121), reads

$$s = \int_{-\infty}^{-Q} \mathrm{d}\Lambda\, \sigma(\Lambda) + \int_{Q}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda) = 2 \int_{Q}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda). \tag{20.123}$$

For $Q = 0$, we have $s = 1$ and $h_c = 2\sqrt{1 + (c')^2} - c$. As follows from (20.79), the band is spin polarized above this critical magnetic field (Phase III).

At $Q \to \infty$, we have $s = 0$ and $h = 0$. Let us introduce the resolvent operator J to the kernel a_2, $(I + J)(I + a_2) = (I + a_2)(I + J) = I$. The function $L_0(\Lambda)$, determined by Eq. (20.118) in the limit $Q \to \infty$, is constant:

$$L_0(\Lambda) = L_0 = \frac{1}{1 + \hat{a}_2(0)} = 1 + \hat{J}(0) = \frac{1}{2}. \tag{20.124}$$

Eqs. (20.113) and (20.119) are solvable by using the Fourier method,

$$\hat{\sigma}_0(\omega) = \frac{1}{2\cosh(c'\omega)} J_0(\omega), \qquad \hat{P}_0(\omega) = \frac{1}{2\cosh(c'\omega)} \frac{J_1(\omega)}{\omega}. \tag{20.125}$$

In the second formula, we used the equality for Bessel functions $[J_0(\omega) + J_2(\omega)]/2 = J_1(\omega)/\omega$. The factor $1/\cosh(c'\omega)$ is a meromorphic function of ω with simple poles at the points

$$\omega_n = \mathrm{i}\frac{\pi}{c}(2n + 1), \qquad n \in Z. \tag{20.126}$$

The large-Λ asymptotic of $\sigma_0(\Lambda)$ and $P_0(\Lambda)$ is determined by the pole at ω_0. Using the residuum theorem, we obtain

$$\sigma_0(\Lambda) \underset{\Lambda\to\infty}{\sim} \frac{1}{c} I_0\left(\frac{\pi}{c}\right) \exp\left(-\frac{\pi}{c}\Lambda\right), \qquad P_0(\Lambda) \underset{\Lambda\to\infty}{\sim} \frac{1}{\pi} I_1\left(\frac{\pi}{c}\right) \exp\left(-\frac{\pi}{c}\Lambda\right), \tag{20.127}$$

where we used that $J_n(\mathrm{i}z) = \mathrm{i}^n I_n(z)$.

Let Q be large, but not infinite, which corresponds to a small magnetic field $h > 0$. The fundamental equations can be solved to the leading order in the deviation of Q from infinity by applying the Wiener-Hopf method [7, 8], in close analogy with Sect. 14. With regard to the large-Λ asymptotic (20.127), we assume that the unknown functions σ and P scale like

$$\sigma(Q + x) \sim \frac{1}{c} I_0\left(\frac{\pi}{c}\right) \mathrm{e}^{-\pi Q/c} T(x), \qquad P(Q + x) \sim \frac{1}{\pi} I_1\left(\frac{\pi}{c}\right) \mathrm{e}^{-\pi Q/c} T(x), \tag{20.128}$$

where $T(x)$ satisfies the Wiener-Hopf integral equation

$$T(x) + \int_0^\infty \mathrm{d}x'\, J(x - x') T(x') = \mathrm{e}^{-\pi x/c}, \qquad x \geq 0. \tag{20.129}$$

The asymptotic form of $L(\Lambda)$ is given by

$$L(Q + x) \sim \frac{1}{2} U(x), \qquad U(x) + \int_0^\infty \mathrm{d}x'\, J(x - x') U(x') = 1, \quad x \geq 0. \tag{20.130}$$

There exists a unique factorization of

$$1 + \hat{a}_2(\omega) = \frac{1}{1 + \hat{J}(\omega)} = F_+(\omega) F_-(\omega) \tag{20.131}$$

by the functions $F_+(\omega)$ and $F_-(\omega)$ which are analytic and nonvanishing in the half-planes Π_+ and Π_-, respectively. The symmetry $J(x) = J(-x)$ implies $F_+(\omega) = F_-(-\omega)$. The $x \to 0^+$ limits of $T(x)$ and $U(x)$ are expressible as

$$\lim_{x\to 0^+} T(x) = F_-(-\mathrm{i}\pi/c), \qquad \lim_{x\to 0^+} U(x) = F_-(0) = F_+(0). \tag{20.132}$$

Consequently,

$$h = \frac{2\pi P(Q)}{L(Q)} = 4I_1\left(\frac{\pi}{c}\right)\mathrm{e}^{-\pi Q/c}\frac{F_-(-\mathrm{i}\pi/c)}{F_+(0)}. \tag{20.133}$$

From Eq. (20.123) we have

$$s = \frac{2}{c}I_0\left(\frac{\pi}{c}\right)\mathrm{e}^{-\pi Q/c}\hat{T}(0). \tag{20.134}$$

Finally, using the relations

$$\hat{T}(0) = \frac{c}{\pi}F_+(0)F_-(-\mathrm{i}\pi/c), \qquad F_+^2(0) = 1 + \hat{a}_2(0) = 2, \tag{20.135}$$

the relationship between h and s is found in the form

$$\frac{h}{s} = \pi\frac{I_1(\pi/c)}{I_0(\pi/c)} + O\left(\frac{1}{Q}\right). \tag{20.136}$$

20.4 Ground-state properties of the attractive Hubbard model

We now describe the ground state in the attractive regime $c < 0$, in the sector with fixed N and M. Each of M Λ-roots remains on the real axis and form a bound state with two wave numbers k_1 and k_2, such that $\bar{k}_1 = k_2$. In the thermodynamic limit $L \to \infty$, the corresponding k-rapidities $\lambda = \sin k$ belong to the 2-string

$$\lambda_1 = \Lambda - \mathrm{i}c' = \sin k_1, \qquad \lambda_2 = \Lambda + \mathrm{i}c' = \sin k_2. \tag{20.137}$$

Since the momentum k is only defined modulo 2π, we can restrict ourselves to $\Re e(k)$ ranging between $-\pi/2$ and $3\pi/2$. Let us take the branch of $\arcsin$ as $-\pi/2 < \Re e(\arcsin x) \leq \pi/2$. We have two possibilities:

$$\begin{array}{l} k_1 = \arcsin(\Lambda - \mathrm{i}c') \\ k_2 = \arcsin(\Lambda + \mathrm{i}c') \end{array}, \qquad \begin{array}{l} E(\Lambda) = -4\Re e\left(\sqrt{1-(\Lambda-\mathrm{i}c')^2}\right) \\ K(\Lambda) = 2\Re e\left(\arcsin(\Lambda - \mathrm{i}c')\right) \end{array}; \tag{20.138}$$

$$\begin{array}{l} k_1 = \pi - \arcsin(\Lambda - \mathrm{i}c') \\ k_2 = \pi - \arcsin(\Lambda + \mathrm{i}c') \end{array}, \qquad \begin{array}{l} E(\Lambda) = 4\Re e\left(\sqrt{1-(\Lambda-\mathrm{i}c')^2}\right) \\ K(\Lambda) = 2\pi - 2\Re e\left(\arcsin(\Lambda - \mathrm{i}c')\right) \end{array}. \tag{20.139}$$

Here, the energy E and the total momentum K were evaluated by using the formulas $E = -2(\cos k_1 + \cos k_2)$ and $K = k_1 + k_2$. The bound state dispersion relations are

$$E(K) = \pm 4\sqrt{(c')^2 + \cos^2(K/2)}. \tag{20.140}$$

The true bound state (20.138) has negative energy. The anti-bound state (20.139), which is an excitation with respect to the bound state, has positive energy.

The remaining $N - 2M$ k's are real. According to the Bethe equations (20.51), they satisfy

$$k_n L = 2\pi I_n - \sum_{\alpha=1}^{M}\theta\left(2(\sin k_n - \Lambda_\alpha)\right), \qquad n = 1, \ldots, N-2M. \tag{20.141}$$

Equations for Λ_α $(\alpha = 1, 2, \ldots, M)$, in which the complex conjugate pairs of wave numbers $k_{\alpha,1}$ and $k_{\alpha,2}$ are eliminated, can be derived in analogy with spin-$\frac{1}{2}$ δ-function fermions (Sect. 10.3.2). The final result is

$$K(\Lambda_\alpha)L = 2\pi J_\alpha - \sum_{\beta=1}^{M} \theta(\Lambda_\alpha - \Lambda_\beta) - \sum_{n=1}^{N-2M} \theta\left(2(\Lambda_\alpha - \sin k_n)\right), \tag{20.142}$$

where the total momentum of the string pair $K(\Lambda)$ is defined in (20.138).

In the sector with the fixed (even) $N = nL$ and zero magnetic field $(M = N/2)$, no unbound particles are present in the ground state. The distribution of particle Λ-roots, $\sigma(\Lambda)$, is restricted to the interval $[-Q, Q]$. In the half filled case $n = 1$, which corresponds to the absolute ground state, $Q \to \infty$. The integral equation for $\sigma(\Lambda)$ then follows from (20.142):

$$\sigma(\Lambda) = \frac{1}{2\pi} K'(\Lambda) - \int_{-\infty}^{\infty} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma(\Lambda'). \tag{20.143}$$

This equation can be solved by the Fourier method. Interestingly, the result coincides with the previous one (20.91). Inserting this solution into the formula for the ground state energy per site

$$e_0 = \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda) E(\Lambda), \tag{20.144}$$

where the energy of the string pair $E(\Lambda)$ is defined by (20.138), we end up with the previous result (20.92) with the substitution $c \to |c|$.

Low-lying excitations at half-filling are basically of two types. Firstly, particle and hole excitations can be created in the fluid of bounded pairs. Secondly, unbound particles can scatter on the ground state fluid of bounded pairs. Dispersion relations for these excitations are derived in Sect. 11.5 of the monograph [9].

20.5 Thermodynamics with strings

The complete thermodynamics of the 1D Hubbard model was derived by Takahashi [10]; for a review, see e.g. Ref. [11]. The thermodynamic Bethe-ansatz method resembles the one for spin-$\frac{1}{2}$ fermions with δ-function interactions, defined on the continuous line (see Sect. 11 for the notation).

There are three types string excitations which contribute to the thermodynamics of the Hubbard model.

- **Strings of Λ-roots:** The Λ-roots can form n-strings $(n = 1, 2, \ldots)$. For a given n, real numbers Λ_α^n $(\alpha = 1, \ldots, M_n)$ denote the string centers. For the given n-string α, the Λ-roots are distributed as follows

$$\Lambda_\alpha^{(n,r)} = \Lambda_\alpha^n + \mathrm{i}c'(n + 1 - 2r), \qquad r = 1, \ldots, n. \tag{20.145}$$

  The same type of excitations occurs in the δ fermion problem, in both repulsive (11.1) and attractive (11.74) regimes.

- **Anti-bound $\Lambda' - k$ strings:** In the attractive regime $c < 0$, it was shown that the real Λ-roots can form a bound state with two k-roots. The bound state (20.138) has an anti-bound excitation (20.139). More generally, in the Hubbard model there exist excitations of n ($n = 1, 2, \ldots$) Λ'-roots and $2n$ wave numbers k. For a given n, ${\Lambda'}_\alpha^n$ ($\alpha = 1, \ldots, M'_n$) denote the real string centers. For the given n-string α, the Λ'-roots are distributed as in (20.145):

$$ {\Lambda'}_\alpha^{(n,r)} = {\Lambda'}_\alpha^n + \mathrm{i}c'(n+1-2r), \qquad r = 1, \ldots, n. \tag{20.146} $$

The corresponding $2n$ k-roots take values

$$ \begin{array}{ll} k_\alpha^{n,1} = \pi - \arcsin({\Lambda'}_\alpha^n - \mathrm{i}nc'), & k_\alpha^{n,2} = \arcsin[{\Lambda'}_\alpha^n - \mathrm{i}(n-2)c'], \\ k_\alpha^{n,3} = \pi - k_\alpha^{n,2}, & k_\alpha^{n,4} = \arcsin[{\Lambda'}_\alpha^n - \mathrm{i}(n-4)c'], \\ k_\alpha^{n,5} = \pi - k_\alpha^{n,4}, & \ldots, \\ \ldots, & k_\alpha^{n,2n-2} = \arcsin[{\Lambda'}_\alpha^n + \mathrm{i}(n-2)c'], \\ k_\alpha^{n,2n-1} = \pi - k_\alpha^{n,2n-2}, & k_\alpha^{n,2n} = \pi - \arcsin({\Lambda'}_\alpha^n + \mathrm{i}nc'). \end{array} \tag{20.147} $$

The energy of this excitation is

$$ E = 4\Re e\left(\sqrt{1 - ({\Lambda'}_\alpha^n - \mathrm{i}nc')}\right). \tag{20.148} $$

The anti-bound state (20.139) corresponds to the special $n = 1$ case. This case resembles the pairs of fermions (11.73) in the attractive δ fermion problem. The excitations with $n > 1$ have no counterparts in that problem. The numbers of Λ and Λ' roots are constrained by $\sum_n nM_n + \sum_n nM'_n = M$.

- **Real independent k-roots:** The remaining $N - 2M'$ ($M' = \sum_n nM'_n$) independent k-roots, which are not bounded with Λ'-roots, are by analogy with δ fermions real. The energy of root k is $E = -2\cos k$.

This classification of excited states is consistent with the number 4^L of eigenstates for the Hubbard Hamiltonian [12].

In close analogy with Sect. 11, the Bethe equations (20.48) and (20.49) can be rewritten as equations containing only real quantities, namely $N - 2M'$ of roots k_j, M' of string centers ${\Lambda'}_\alpha^n$ and $M - M'$ of string centers Λ_α^n:

$$ \exp(\mathrm{i}k_j L) = \prod_{(n,\alpha)} e_n(\sin k_j - \Lambda_\alpha^n) \prod_{(n,\alpha)} e_n(\sin k_j - {\Lambda'}_\alpha^n), \tag{20.149} $$

$$ \begin{aligned} \exp(\mathrm{i}\sum_{s=1}^{2n} k_\alpha^{n,s} L) &= \exp\left(-L\left[\arcsin({\Lambda'}_\alpha^n - \mathrm{i}nc') + \arcsin({\Lambda'}_\alpha^n + \mathrm{i}nc')\right]\right) \\ &= -\prod_{j=1}^{N-2M'} e_n({\Lambda'}_\alpha^n - \sin k_j) \prod_{(m,\beta)} E_{nm}({\Lambda'}_\alpha^n - {\Lambda'}_\beta^m), \end{aligned} \tag{20.150} $$

$$\prod_{j=1}^{N-2M'} e_n(\Lambda_\alpha^n - \sin k_j) = -\prod_{(m,\beta)} E_{nm}(\Lambda_\alpha^n - \Lambda_\beta^m). \tag{20.151}$$

Taking the logarithm of these equations results in

$$k_j L = 2\pi I_j - \sum_{(n,\alpha)} \theta_n(\sin k_j - \Lambda_\alpha^n) - \sum_{(n,\alpha)} \theta_n(\sin k_j - \Lambda'^n_\alpha), \tag{20.152}$$

$$\begin{aligned} &L\left[\arcsin(\Lambda'^n_\alpha - \mathrm{i}nc') + \arcsin(\Lambda'^n_\alpha + \mathrm{i}nc')\right] = 2\pi J'^n_\alpha \\ &+ \sum_{j=1}^{N-2M'} \theta_n(\Lambda'^n_\alpha - \sin k_j) + \sum_{(m,\beta)} \Theta_{nm}(\Lambda'^n_\alpha - \Lambda'^m_\beta), \end{aligned} \tag{20.153}$$

$$\sum_{j=1}^{N-2M'} \theta_n(\Lambda_\alpha^n - \sin k_j) = 2\pi J_\alpha^n + \sum_{(m,\beta)} \Theta_{nm}(\Lambda_\alpha^n - \Lambda_\beta^m). \tag{20.154}$$

Here, I_j, J_α^n and J'^n_α are integers or half-odd integers, constrained by

$$\begin{aligned} &|J_\alpha^n| < \tfrac{1}{2}\left(N - 2M' - \textstyle\sum_{m=1}^{\infty} t_{nm} M'_m\right), \\ &|J'^n_\alpha| < \tfrac{1}{2}\left(L - N + 2M' - \textstyle\sum_{m=1}^{\infty} t_{nm} M'_m\right). \end{aligned} \tag{20.155}$$

In the thermodynamic limit, let $\rho(k)$, $\sigma_n(\Lambda)$ and $\sigma'_n(\Lambda)$ be the particle distribution functions of k-roots, n-string Λ and Λ' centers, respectively. The corresponding hole distribution functions will be denoted as $\tilde{\rho}(k)$, $\tilde{\sigma}_n(\Lambda)$ and $\tilde{\sigma}'_n(\Lambda)$. Eqs. (20.152)–(20.154) imply the following constraints among the particle and hole distribution functions:

$$\frac{1}{2\pi} = \rho(k) + \tilde{\rho}(k) - \cos k \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, a_n(\sin k - \Lambda)\left[\sigma_n(\Lambda) + \sigma'_n(\Lambda)\right], \tag{20.156}$$

$$\int_{-\pi}^{\pi} \mathrm{d}k\, a_n(\Lambda - \sin k)\rho(k) = \tilde{\sigma}_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\Lambda), \tag{20.157}$$

$$\begin{aligned} &\frac{1}{\pi}\Re e\left(\frac{1}{\sqrt{1-(\Lambda - \mathrm{i}nc')^2}}\right) - \int_{-\pi}^{\pi} \mathrm{d}k\, a_n(\Lambda - \sin k)\rho(k) \\ &\qquad = \tilde{\sigma}'_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma'_m(\Lambda). \end{aligned} \tag{20.158}$$

The Gibbs free energy per site is given by

$$g = -\frac{1}{\beta}\frac{S}{L} + \frac{E}{L} - \mu\frac{N}{L}, \tag{20.159}$$

where

$$\begin{aligned}
\frac{E}{L} &= -2\int_{-\pi}^{\pi} \mathrm{d}k\, \cos k\rho(k) - h\left(\frac{N}{L} - 2\frac{M}{L}\right) \\
&\quad +4\sum_{n=1}^{\infty}\int \mathrm{d}\Lambda\, \Re e\left(\sqrt{1-(\Lambda - \mathrm{i}nc')^2}\right)\sigma_n'(\Lambda), \qquad (20.160)\\
\frac{N}{L} &= \int_{-\pi}^{\pi} \mathrm{d}k\, \rho(k) + \sum_{n=1}^{\infty} 2n \int \mathrm{d}\Lambda\, \sigma_n'(\Lambda), \qquad (20.161)\\
\frac{M}{L} &= \sum_{n=1}^{\infty} n \int \mathrm{d}\Lambda\, \left[\sigma_n(\Lambda) + \sigma_n'(\Lambda)\right], \qquad (20.162)\\
\frac{S}{L} &= \int_{-\pi}^{\pi} \mathrm{d}k\, \left[(\rho+\tilde\rho)\ln(\rho+\tilde\rho) - \rho\ln\rho - \tilde\rho\ln\tilde\rho\right] \\
&\quad +\sum_{n=1}^{\infty}\int \mathrm{d}\Lambda\, \left[(\sigma_n+\tilde\sigma_n)\ln(\sigma_n+\tilde\sigma_n) - \sigma_n\ln\sigma_n - \tilde\sigma_n\ln\tilde\sigma_n\right] \\
&\quad +\sum_{n=1}^{\infty}\int \mathrm{d}\Lambda\, \left[(\sigma_n'+\tilde\sigma_n')\ln(\sigma_n'+\tilde\sigma_n') - \sigma_n'\ln\sigma_n' - \tilde\sigma_n'\ln\tilde\sigma_n'\right]. \qquad (20.163)
\end{aligned}$$

The variational condition $\delta g = 0$, under the constraints (20.156)–(20.158), implies an infinite set of coupled equations for the ratios $\tilde\rho/\rho \equiv \exp(\beta\epsilon)$, $\tilde\sigma_n/\sigma_n \equiv \eta_n$ and $\tilde\sigma_n'/\sigma_n' \equiv \eta_n'$:

$$\begin{aligned}
\beta\epsilon(k) &= -\beta(2\cos k + \mu + h) \\
&\quad +\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, a_n(\sin k - \Lambda)\ln\left(\frac{1+\eta_n'^{-1}(\Lambda)}{1+\eta_n^{-1}(\Lambda)}\right), \qquad (20.164)\\
\ln[1+\eta_n(\Lambda)] &= 2n\beta h - \int_{-\pi}^{\pi} \mathrm{d}k\, a_n(\Lambda - \sin k)\ln[1+\mathrm{e}^{-\beta\epsilon(k)}]\cos k \\
&\quad +\sum_{m=1}^{\infty} A_{nm} * \ln[1+\eta_m^{-1}(\Lambda)], \qquad (20.165)\\
\ln[1+\eta_n'(\Lambda)] &= \beta\left[4\Re e\left(\sqrt{1-(\Lambda-\mathrm{i}nc')^2}\right) - 2n\mu\right] \\
&\quad -\int_{-\pi}^{\pi} \mathrm{d}k\, a_n(\Lambda - \sin k)\ln[1+\mathrm{e}^{-\beta\epsilon(k)}]\cos k \\
&\quad +\sum_{m=1}^{\infty} A_{nm} * \ln[1+\eta_m'^{-1}(\Lambda)]. \qquad (20.166)
\end{aligned}$$

For the pressure $P = -g$ we have the expression

$$\begin{aligned}
\beta P &= \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, \ln\left[1+\mathrm{e}^{-\beta\epsilon(k)}\right] \\
&\quad +\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}\Lambda}{\pi}\, \Re e\left(\frac{1}{\sqrt{1-(\Lambda-\mathrm{i}nc')^2}}\right)\ln\left[1+\eta_n'^{-1}(\Lambda)\right]. \qquad (20.167)
\end{aligned}$$

Using matrix Eqs. (11.29)–(11.33) and (11.47), the infinite chain of coupled equations (20.164)–(20.166) is transformed to

$$\begin{aligned}
\beta\epsilon(k) &= \beta\kappa(k) + \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, s(\sin k - \Lambda) \ln\left(\frac{1+\eta_1'(\Lambda)}{1+\eta_1(\Lambda)}\right), && (20.168)\\
\ln\eta_1(\Lambda) &= s * \ln[1+\eta_2(\Lambda)] \\
&\quad - \int_{-\pi}^{\pi} \mathrm{d}k\, s(\Lambda - \sin k) \ln[1+\mathrm{e}^{-\beta\epsilon(k)}] \cos k, && (20.169)\\
\ln\eta_1'(\Lambda) &= s * \ln[1+\eta_2'(\Lambda)] \\
&\quad - \int_{-\pi}^{\pi} \mathrm{d}k\, s(\Lambda - \sin k) \ln[1+\mathrm{e}^{\beta\epsilon(k)}] \cos k, && (20.170)\\
\ln\eta_n(\Lambda) &= s * \ln\left\{[1+\eta_{n-1}(\Lambda)][1+\eta_{n+1}(\Lambda)]\right\}, \qquad n \geq 2, && (20.171)\\
\ln\eta_n'(\Lambda) &= s * \ln\left\{[1+\eta_{n-1}'(\Lambda)][1+\eta_{n+1}'(\Lambda)]\right\}, \qquad n \geq 2, && (20.172)\\
\lim_{n\to\infty} \frac{\ln\eta_n(\Lambda)}{n} &= 2\beta h, && (20.173)\\
\lim_{n\to\infty} \frac{\ln\eta_n'(\Lambda)}{n} &= 2\beta(c-\mu), && (20.174)
\end{aligned}$$

where $\kappa(k)$ is defined by

$$\kappa(k) \equiv -2\cos k - 4\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, s(\sin k - \Lambda) \Re e\left(\sqrt{1-(\Lambda - \mathrm{i}c')^2}\right). \qquad (20.175)$$

These TBA equations can be solved numerically, or analytically in special limits.

• **The limit** $T \to 0$**:** The last terms in Eqs. (20.169) and (20.170) can be re-expressed as

$$-\int_{-\pi/2}^{\pi/2} \mathrm{d}k\, s(\Lambda - \sin k) \ln\left[\frac{1+\mathrm{e}^{-\beta\epsilon(k)}}{1+\mathrm{e}^{-\beta\epsilon(\pi-k)}}\right] \cos k \qquad (20.176)$$

and

$$-\int_{-\pi/2}^{\pi/2} \mathrm{d}k\, s(\Lambda - \sin k) \ln\left[\frac{1+\mathrm{e}^{\beta\epsilon(k)}}{1+\mathrm{e}^{\beta\epsilon(\pi-k)}}\right] \cos k, \qquad (20.177)$$

respectively. The function $\kappa(k)$ (20.175) satisfies the relation $\kappa(k) - \kappa(\pi - k) = -4\cos k$. Thus for $|k| < \pi/2$ we have $\epsilon(k) < \epsilon(\pi - k)$. Consequently, the last term in (20.169) is negative and the last one in (20.170) is positive. Defining

$$\beta\epsilon_n(\Lambda) = \ln\eta_n(\Lambda), \qquad \beta\epsilon_n'(\Lambda) = \ln\eta_n'(\Lambda), \qquad n = 1, 2, \ldots, \qquad (20.178)$$

we find that $\epsilon_2, \epsilon_3, \ldots$ and $\epsilon_1', \epsilon_2', \ldots$ are always positive, while the signs of $\epsilon(k)$ and $\epsilon_1(\Lambda)$ can be either positive or negative. This fact is important in the limit of zero temperature. Let us denote by $k = \pm q$ and $\Lambda = \pm Q$ the points at which $\epsilon(k)$ and $\epsilon_1(\Lambda)$ change sign, respectively. Knowing that $\epsilon(k) < 0$ for $|k| < q$ and $\epsilon_1(\Lambda) < 0$ for $|\Lambda| < Q$, using (20.164) and (20.165) taken at $n = 1$, we end up with the ground-state integral equations for dressed energies (20.57) and (20.58).

• **The limit** $c \to 0^+$**:** In this limit, we define

$$\epsilon_-(\Lambda) \equiv \epsilon(k = \arcsin\Lambda), \qquad \epsilon_+(\Lambda) \equiv \epsilon(k = \pi - \arcsin\Lambda), \tag{20.179}$$

where $|\Lambda| \leq 1$ (we recall that $|\arcsin\Lambda| \leq \pi/2$). The function $s(x)$ (11.33) can be replaced by $\delta(x)/2$ in the limit $c \to 0^+$. The set of integral equations (20.168)–(20.174), considered with the representations (20.176) and (20.177) of integrals over k, then becomes

$$\begin{aligned}
\beta\epsilon_\pm &= (-2 \pm 2)\beta\sqrt{1-\Lambda^2} + \frac{1}{2}\ln\left(\frac{1+\eta_1'}{1+\eta_1}\right), && (20.180)\\
\ln\eta_1 &= \frac{1}{2}\ln(1+\eta_2) + \frac{1}{2}\ln\left(\frac{1+\mathrm{e}^{-\beta\epsilon_+}}{1+\mathrm{e}^{-\beta\epsilon_-}}\right), && (20.181)\\
\ln\eta_1' &= \frac{1}{2}\ln(1+\eta_2') + \frac{1}{2}\ln\left(\frac{1+\mathrm{e}^{\beta\epsilon_+}}{1+\mathrm{e}^{\beta\epsilon_-}}\right), && (20.182)\\
\ln\eta_n &= \frac{1}{2}\ln\left[(1+\eta_{n-1})(1+\eta_{n+1})\right], \qquad n \geq 2, && (20.183)\\
\ln\eta_n' &= \frac{1}{2}\ln\left[(1+\eta_{n-1}')(1+\eta_{n+1}')\right], \qquad n \geq 2, && (20.184)\\
\lim_{n\to\infty}\frac{\ln\eta_n}{n} &= 2\beta h, && (20.185)\\
\lim_{n\to\infty}\frac{\ln\eta_n'}{n} &= -2\beta\mu. && (20.186)
\end{aligned}$$

Eqs. (20.183)–(20.186) are difference equations, their general solution reads

$$\begin{aligned}
&\eta_n = f^2(n) - 1, \qquad f(n) = \frac{aw^n - a^{-1}w^{-n}}{w - w^{-1}}, \qquad w = \mathrm{e}^{-\beta h};\\
&\eta_n' = g^2(n) - 1, \qquad g(n) = \frac{bz^n - b^{-1}z^{-n}}{z - z^{-1}}, \qquad z = \mathrm{e}^{\beta\mu}, && (20.187)
\end{aligned}$$

where a and b are free parameters. Substituting the general solution into (20.180)–(20.182) leads to

$$\begin{aligned}
&\mathrm{e}^{\beta\epsilon_+} = \frac{g(1)}{f(1)}, \qquad \mathrm{e}^{\beta\epsilon_-} = \frac{1}{x^2}\frac{g(1)}{f(1)}, \qquad x \equiv \exp\left(2\beta\sqrt{1-\Lambda^2}\right);\\
&f^2(0) = \frac{1+\mathrm{e}^{-\beta\epsilon_+}}{1+\mathrm{e}^{-\beta\epsilon_-}}, \qquad g^2(0) = \frac{1+\mathrm{e}^{\beta\epsilon_+}}{1+\mathrm{e}^{\beta\epsilon_-}}. && (20.188)
\end{aligned}$$

The solution of these relations with respect to a and b reads

$$\begin{aligned}
a &= \sqrt{\frac{(1+x^{-1}wz)(1+x^{-1}wz^{-1})}{(1+x^{-1}w^{-1}z)(1+x^{-1}w^{-1}z^{-1})}},\\
b &= \sqrt{\frac{(1+xwz)(1+xw^{-1}z)}{(1+xwz^{-1})(1+xw^{-1}z^{-1})}}. && (20.189)
\end{aligned}$$

It is easy to derive from (20.167) taken with $c' = 0$ that

$$\beta P = \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\ln\left[\left(1+\mathrm{e}^{\beta(2\cos k+\mu-h)}\right)\left(1+\mathrm{e}^{\beta(2\cos k+\mu+h)}\right)\right]. \tag{20.190}$$

This is the result for the pressure of free electrons on the discrete chain.

• **The limit $c \to \infty$:** In this limit $\eta_n' = \infty$ for all $n = 1, 2, \ldots$. The function $s(x)$ becomes infinitely wide. Similarly as for fermions with δ-function interactions on the continuous line, η_n become Λ-independent and the TBA equations simplify to (11.58) with the solution (11.59). Thus,

$$\epsilon(k) = -2\cos k - \mu - \frac{1}{2\beta}\ln(1+\eta_1) = -2\cos k - \mu - \ln[2\cosh(\beta h)]. \tag{20.191}$$

The pressure (20.167) is given by

$$\beta P = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \ln\left[1 + 2\cosh(\beta h)\mathrm{e}^{\beta(\mu + 2\cos k)}\right]. \tag{20.192}$$

21 Kondo effect

Dilute magnetic alloys are composed of a small amount of magnetic impurities dissolved in a non-magnetic metal. The impurities are represented by localized spins which interact with the conduction-band electrons via a spin exchange. At low temperatures, where the standard perturbation theory is not applicable, an anomalous scattering of conduction electrons on the impurities leads to many interesting phenomena known as the Kondo effect [13]. There are many microscopic models of dilute magnetic alloys, which are completely integrable; see e.g. reviews [14, 15]. These include the $s-d$ exchange model and the degenerate exchange model of a single impurity, introduced by Vousovskii [16] and Zener [17], the Anderson model and the degenerate Anderson model [18, 19].

Here, we shall concentrate on the $s-d$ exchange (Kondo) model in an external magnetic field H. At a given temperature T, this model was solved by using the Bethe ansatz method by Andrei [20] and Wiegmann [21]. The TBA equations are analyzed in the ultraviolet regime (large H or high T) and in the infrared regime (small H or low T). In the ultraviolet limit, the impurity behaves like an almost free spin, its properties are described by an effective weakly coupled theory. In the infrared limit, the impurity is completely ($s=\frac{1}{2}$) or partially ($s>\frac{1}{2}$) screened, its properties are described by another effective (strongly coupled) Fermi liquid theory. The crossover from one regime to another, driven by the temperature of magnetic field, is known as the Kondo effect.

21.1 Hamiltonian

The $s-d$ exchange model describes the interaction of the conduction band of a 3D metal with one impurity of arbitrary spin $\mathbf{S}=(S^x,S^y,S^z)$ (the eigenvalues of S^z will be denoted by $\mathfrak{s}=-s,-s+1,\ldots,s$) localized at the origin $\mathbf{r}=\mathbf{0}$. In the second quantization, the conduction band is described by the Hamiltonian

$$H_0=\sum_{\mathbf{k},\sigma}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}, \tag{21.1}$$

where $c_{\mathbf{k}\sigma}$ ($c^\dagger_{\mathbf{k}\sigma}$) is the annihilation (creation) operator of an electron with Fourier momentum $\mathbf{k}$, energy $\epsilon_{\mathbf{k}}$ and spin-$\frac{1}{2}$ component $\sigma\in\{-\frac{1}{2},\frac{1}{2}\}$. The conduction band is coupled to the spin-s impurity via the exchange interaction

$$H_I=\frac{J}{2}\sum_{\sigma,\sigma'}\Psi^\dagger_\sigma(\mathbf{r}=0)\boldsymbol{\sigma}_{\sigma\sigma'}\Psi_{\sigma'}(\mathbf{r}=0)\cdot\mathbf{S}=\frac{J}{2}\sum_{\substack{\mathbf{k},\mathbf{k}'\\ \sigma,\sigma'}}c^\dagger_{\mathbf{k}\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{\mathbf{k}'\sigma'}\cdot\mathbf{S}, \tag{21.2}$$

where $\boldsymbol{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$ denotes the Pauli matrices. Since the system is rotationally invariant, it is useful to expand the electron annihilation and creation operators in the basis of the spherical functions:

$$c_{\mathbf{k}\sigma}=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\mathbf{k}/k)c_{klm,\sigma},\qquad c^\dagger_{\mathbf{k}\sigma}=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y^*_{lm}(\mathbf{k}/k)c^\dagger_{klm,\sigma}. \tag{21.3}$$

We assume that from the angular modes only the s-wave modes with $l = m = 0$ have nonzero coupling to the impurity; the consideration of higher orbital modes would lead to the so-called Multi-Channel Kondo model.

Let us further restrict ourselves to momenta k close to the Fermi surface, $k = k_F + p$ with a cut-off of the order of k_F for new momenta p, and consider the linear dispersion law

$$\epsilon_k \sim \varepsilon_{\rm F} + v_F p. \tag{21.4}$$

The linearization is adequate only when all energy scales (like temperature, magnetic field, excitation energies, etc.) are small compared to the cut-off. Consequently, only "universal quantities", which characterize low-energy properties of the system and are independent of the cut-off, will be studied. We shift the energy by $\varepsilon_{\rm F}$, set $v_F = 1$ and leave in the free-electron H_0 only the relevant electrons with $l = m = 0$. Using the notation $c_{k_F+p,00,\sigma} \equiv c_{p\sigma}$ and $c^\dagger_{k_F+p,00,\sigma} \equiv c^\dagger_{p\sigma}$, the total Hamiltonian $H = H_0 + H_I$ reads

$$H = \sum_{p,\sigma} p c^\dagger_{p\sigma} c_{p\sigma} + \frac{J}{2} \sum_{\substack{p,p'\\ \sigma,\sigma'}} c^\dagger_{p\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{p'\sigma'} \cdot \mathbf{S}. \tag{21.5}$$

This Hamiltonian is effectively one-dimensional. In the coordinate representation $c_\sigma(x) = \int \mathrm{d}p\, \exp(\mathrm{i}px) c_{p\sigma}$, it takes the form

$$H = \int \mathrm{d}x \left[-\mathrm{i} \sum_\sigma c^\dagger_\sigma(x) \frac{\partial}{\partial x} c_\sigma(x) + \frac{J}{2} \delta(x) \sum_{\sigma,\sigma'} c^\dagger_\sigma(x) \boldsymbol{\sigma}_{\sigma\sigma'} c_{\sigma'}(x) \cdot \mathbf{S} \right]. \tag{21.6}$$

In the first quantization, the Schrödinger equation for N electrons $(\sigma_1, x_1), \ldots, (\sigma_N, x_N)$ and one impurity at $x_0 = 0$ with $\mathfrak{s} \in \{-s, -s+1, \ldots, s\}$ reads

$$\left(-\mathrm{i} \sum_{j=1}^N \frac{\partial}{\partial x_j} - E \right) \psi_{\sigma_1 \ldots \sigma_N; \mathfrak{s}}(x_1, \ldots, x_N) + \frac{J}{2} \sum_{j=1}^N \delta(x_j) \times \sum_{\sigma'_j, \mathfrak{s}'} \left(\boldsymbol{\sigma}_{\sigma_j \sigma'_j} \cdot \mathbf{S}_{\mathfrak{s}\mathfrak{s}'} \right) \psi_{\sigma_1 \ldots \sigma'_j \ldots \sigma_N; \mathfrak{s}'}(x_1, \ldots, x_N) = 0. \tag{21.7}$$

21.2 Electron-impurity and electron-electron scattering matrices

Let us first solve the Schrödinger Eq. (21.7) for a single electron interacting with the impurity at $x_0 = 0$:

$$\left(-\mathrm{i} \frac{\mathrm{d}}{\mathrm{d}x} - E \right) \psi_{\sigma;\mathfrak{s}}(x) + \frac{J}{2} \delta(x) \sum_{\sigma',\mathfrak{s}'} (\boldsymbol{\sigma}_{\sigma\sigma'} \cdot \mathbf{S}_{\mathfrak{s}\mathfrak{s}'}) \psi_{\sigma';\mathfrak{s}'}(x) = 0. \tag{21.8}$$

The δ-potential in this equation can be replaced by a smooth potential $V_\varepsilon(x)$ such that

$$\lim_{\varepsilon \to 0} V_\varepsilon(x) = \frac{J}{2} \delta(x). \tag{21.9}$$

The wavefunction is searched in the form $\psi_{\sigma;\mathfrak{s}}(x) = \exp(\mathrm{i}kx)A_{\sigma;\mathfrak{s}}(x)$. Setting $E = k$, Eq. (21.8) reduces to the ordinary differential equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}A_{\sigma;\mathfrak{s}}(x) = V_\varepsilon(x)\sum_{\sigma',\mathfrak{s}'}(\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\mathbf{S}_{\mathfrak{s}\mathfrak{s}'})A_{\sigma';\mathfrak{s}'}(x), \tag{21.10}$$

whose explicit solution for the A-matrix reads

$$A_{\sigma;\mathfrak{s}}(x) = \sum_{\sigma',\mathfrak{s}'}\left\{\exp\left[-\mathrm{i}\boldsymbol{\sigma}\cdot\mathbf{S}\int_y^x \mathrm{d}x'\,V_\varepsilon(x')\right]\right\}_{\sigma'\mathfrak{s}'}^{\sigma\mathfrak{s}} A_{\sigma';\mathfrak{s}'}(y). \tag{21.11}$$

Taking the limit $\varepsilon \to 0$ we find

$$A_{\sigma;\mathfrak{s}}(x>0) = \sum_{\sigma',\mathfrak{s}'}(S_{10})^{\sigma\mathfrak{s}}_{\sigma'\mathfrak{s}'}\,A_{\sigma';\mathfrak{s}'}(x<0), \qquad S_{10} = \exp\left(-\mathrm{i}\frac{J}{2}\boldsymbol{\sigma}_1\cdot\mathbf{S}_0\right), \tag{21.12}$$

where the subscripts 1 and 0 correspond to the electron and the impurity, respectively. The scattering matrix S_{10} can be written in a more convenient form by using the expansion

$$S_{10} = \exp\left(-\mathrm{i}\frac{J}{2}\boldsymbol{\sigma}_1\cdot\mathbf{S}_0\right) = w_0' + 2w'\boldsymbol{\sigma}_1\cdot\mathbf{S}_0, \tag{21.13}$$

where w_0' and w' are some functions of J. To find these functions we take advantage of the fact that the total spin $\boldsymbol{\sigma}/2 + \mathbf{S}$ can acquire the values $s+\frac{1}{2}$ and $s-\frac{1}{2}$. In the former case, since

$$\begin{aligned}\left(\frac{\boldsymbol{\sigma}}{2}+\mathbf{S}\right)\cdot\left(\frac{\boldsymbol{\sigma}}{2}+\mathbf{S}\right)\psi &\equiv \left(\frac{\boldsymbol{\sigma}^2}{4}+\boldsymbol{\sigma}\cdot\mathbf{S}+\mathbf{S}^2\right)\psi \\ &= \left(s+\frac{1}{2}\right)\left(s+\frac{3}{2}\right)\psi\end{aligned} \tag{21.14}$$

and $\boldsymbol{\sigma}^2\psi = 3\psi$, $\mathbf{S}^2\psi = s(s+1)\psi$, we have $\boldsymbol{\sigma}\cdot\mathbf{S}\psi = s\psi$. Similarly, if the total spin equals to $s-\frac{1}{2}$, we find $\boldsymbol{\sigma}\cdot\mathbf{S}\psi = -(s+1)\psi$. Thus w_0' and w' are given by

$$\exp\left(-\mathrm{i}\frac{Js}{2}\right) = w_0' + 2sw', \qquad \exp\left(\mathrm{i}\frac{J(s+1)}{2}\right) = w_0' - 2(s+1)w'. \tag{21.15}$$

Now we consider two electron in presence of the impurity fixed at $x_0 = 0$. The scattering of electron $j = 1, 2$ on the impurity 0 is again described by the matrix S_{j0} defined for $j = 1$ in (21.13). Due to absence of interaction terms between electrons, a problem of uniqueness arises in the scattering of two electrons. Let the electrons be far away from the impurity, say $x_1, x_2 < 0$, with the "kinetic" Hamiltonian $H = -\mathrm{i}(\partial_1+\partial_2)$. We are allowed to consider a basis of free antisymmetric eigenstates (the impurity state $\mathfrak{s}$ is fixed)

$$\begin{aligned}\psi_{\sigma_1\sigma_2}(x_1,x_2) &= \mathrm{e}^{\mathrm{i}(k_1x_1+k_2x_2)}\left[A_{\sigma_1\sigma_2}\theta(x_1-x_2)+(S_{12}A)_{\sigma_1\sigma_2}\theta(x_2-x_1)\right] \\ &- \mathrm{e}^{\mathrm{i}(k_2x_1+k_1x_2)}\left[A_{\sigma_2\sigma_1}\theta(x_2-x_1)+(S_{12}A)_{\sigma_2\sigma_1}\theta(x_1-x_2)\right].\end{aligned} \tag{21.16}$$

Since $H\theta(x_1-x_2) = 0$, this function is the solution of the Schrödinger equation with the eigenvalue $E = k_1+k_2$ for *any choice* of the scattering matrix S_{12}. This freedom is related to

the degeneracy of E in wave numbers $k_1 \to k_1 + p$ and $k_2 \to k_2 - p$ for any p, which allows us to sum freely the basis over p to generate (21.16). Our motivation for the choice of S_{12} comes from the scattering of the two electrons by the impurity. There exist two different ways how to go from the initial state $x_1 \le x_2 \le 0$ to the final state $0 \le x_2 \le x_1$. The first path

$$x_1 \le x_2 \le 0 \to x_1 \le 0 \le x_2 \to 0 \le x_1 \le x_2 \to 0 \le x_2 \le x_1$$

transforms A to $S_{12}S_{10}S_{20}A$. The second path

$$x_1 \le x_2 \le 0 \to x_2 \le x_1 \le 0 \to x_2 \le 0 \le x_1 \to 0 \le x_2 \le x_1$$

transforms A to $S_{20}S_{10}S_{12}A$. Because the result must be the same in both cases, we end up with the spectral-independent YBE of type

$$S_{12}S_{10}S_{20} = S_{20}S_{10}S_{12}. \tag{21.17}$$

This equation is fulfilled if we identify S_{12} with the permutation operator,

$$S_{12} = \mathcal{P}_{12} = \frac{1}{2}\left(1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\right). \tag{21.18}$$

Note that the scattering matrices do not depend on the wave numbers k_1 and k_2.

The extension of the formalism to N particles is straightforward. The scattering of the particle $j = 1, \ldots, N$ on the impurity 0 is described by the matrix S_{j0} which is the obvious extension of (21.13). The two-electron scattering matrices are again $S_{jk} = \mathcal{P}_{jk}$. The scattering matrices satisfy two kinds of three-particle YBE:

$$S_{jk}S_{j0}S_{k0} = S_{k0}S_{j0}S_{jk} \qquad j,k = 1,\ldots,N, \tag{21.19}$$

$$S_{jk}S_{jl}S_{kl} = S_{kl}S_{jl}S_{jk} \qquad j,k,l = 1,\ldots,N. \tag{21.20}$$

The energy is the sum of electron momenta, $E = \sum_{j=1}^{N} k_j$.

In order to apply QISM, we need YBE containing spectral parameters. Our strategy is to assume that YBE (21.19) and (21.20) correspond to some special cases of the spectral-dependent YBE

$$S_{jk}(\lambda)S_{j0}(\lambda+\mu)S_{k0}(\mu) = S_{k0}(\mu)S_{j0}(\lambda+\mu)S_{jk}(\lambda) \qquad j,k = 1,\ldots,N, \tag{21.21}$$

$$S_{jk}(\lambda)S_{jl}(\lambda+\mu)S_{kl}(\mu) = S_{kl}(\mu)S_{jl}(\lambda+\mu)S_{jk}(\lambda) \qquad j,k,l = 1,\ldots,N. \tag{21.22}$$

Eq. (21.19) is identified from (21.21) if we set $\lambda = 0$ and say $\mu = 1$, Eq. (21.20) is identified from (21.22) if we set $\lambda = \mu = 0$. Thus,

$$\begin{aligned} S_{j0} &\equiv S_{j0}(\lambda_j - \lambda_0) = S_{j0}(1), \\ S_{jk} &\equiv S_{jk}(\lambda_j - \lambda_k) = S_{jk}(0), \end{aligned} \qquad j,k = 1,\ldots,N. \tag{21.23}$$

A simple choice of spectral parameters for the impurity and electrons is

$$\lambda_0 = -1, \qquad \lambda_j = 0 \qquad j = 1,\ldots,N. \tag{21.24}$$

Being motivated by the special $\lambda = 1$ case (21.13), the λ-dependent electron-impurity scattering matrix is assumed to be in the form

$$[S_{j0}(\lambda)]^{\sigma_j \mathfrak{s}}_{\sigma_j' \mathfrak{s}'} = w_0'(\lambda)\delta(\sigma_j, \sigma_j')\delta(\mathfrak{s}, \mathfrak{s}') + 2w'(\lambda)\boldsymbol{\sigma}_{\sigma_j \sigma_j'} \cdot \mathbf{S}_{\mathfrak{s}\mathfrak{s}'} \tag{21.25}$$

($j = 1, \ldots, N$). Taking into account the relations (21.15), the $\lambda = 1$ case implies the "boundary" conditions

$$\begin{aligned} w_0'(1) &= \frac{1}{2s+1}\left[(s+1)\mathrm{e}^{-\mathrm{i}Js/2} + s\mathrm{e}^{\mathrm{i}J(s+1)/2}\right], \\ w'(1) &= \frac{1}{2(2s+1)}\left[\mathrm{e}^{-\mathrm{i}Js/2} - \mathrm{e}^{\mathrm{i}J(s+1)/2}\right]. \end{aligned} \tag{21.26}$$

Similarly, with regard to the special $\lambda = 0$ case (21.18), the λ-dependent electron-electron scattering matrix is searched in the form

$$[S_{jk}(\lambda)]^{\sigma_j\sigma_k}_{\sigma_j'\sigma_k'} = w_0(\lambda)\delta(\sigma_j, \sigma_j')\delta(\sigma_k, \sigma_k') + w(\lambda)\boldsymbol{\sigma}_{\sigma_j\sigma_j'} \cdot \boldsymbol{\sigma}_{\sigma_k\sigma_k'} \tag{21.27}$$

($j, k = 1, \ldots, N$). The case $\lambda = 0$ implies the boundary conditions

$$w_0(0) = \frac{1}{2}, \qquad w(0) = \frac{1}{2}. \tag{21.28}$$

It is convenient to introduce

$$\begin{array}{lll} a(\lambda) = w_0(\lambda) + w(\lambda), & b(\lambda) = w_0(\lambda) - w(\lambda), & c(\lambda) = 2w(\lambda), \\ a'(\lambda) = w_0'(\lambda) + w'(\lambda), & b'(\lambda) = w_0'(\lambda) - w'(\lambda), & c'(\lambda) = 2w'(\lambda). \end{array} \tag{21.29}$$

We shall need the following boundary conditions

$$a(0) = 1, \qquad a'(1) = \frac{1}{2s+1}\left[\left(s + \frac{3}{2}\right)\mathrm{e}^{-\mathrm{i}Js/2} + \left(s - \frac{1}{2}\right)\mathrm{e}^{\mathrm{i}J(s+1)/2}\right]. \tag{21.30}$$

Substituting the scattering matrices (21.25) and (21.27) into YBE (21.21) and (21.22), we obtain the following equalities

$$h(\lambda) \equiv \frac{b(\lambda)}{c(\lambda)} = \frac{b'(\lambda)}{c'(\lambda)}, \qquad h(\lambda) + h(\mu) = h(\lambda + \mu). \tag{21.31}$$

The general solution of these equations is $h(\lambda) = \lambda/(-\mathrm{i}g)$, where g is a parameter. Taking $\lambda = 1$, we find that

$$g = \frac{2}{2s+1}\tan\left[\frac{J}{4}(2s+1)\right]. \tag{21.32}$$

Simultaneously, we have

$$\begin{aligned} b(\lambda) &= \frac{\lambda}{\lambda - \mathrm{i}g}a(\lambda), \qquad & c(\lambda) &= \frac{-\mathrm{i}g}{\lambda - \mathrm{i}g}a(\lambda) \\ b'(\lambda) &= \frac{\lambda}{\lambda - \mathrm{i}g}a'(\lambda), \qquad & c'(\lambda) &= \frac{-\mathrm{i}g}{\lambda - \mathrm{i}g}a'(\lambda). \end{aligned} \tag{21.33}$$

21.3 Inhomogeneous QISM

Let the system of N electrons and one impurity be placed on the line of length L. Imposing periodic boundary conditions for the wavefunction leads to N eigenvalue equations for electron momenta (see Sect. 9)

$$\exp(-\mathrm{i}k_j L)A = \mathrm{T}_j A \qquad j = 1, \ldots, N. \tag{21.34}$$

The operator T_j is defined by

$$T_j = T(\lambda = \lambda_j; \lambda_0, \ldots, \lambda_N), \tag{21.35}$$

where the transfer matrix T is the trace of the monodromy matrix $\mathcal{T}_\xi$ in the auxiliary spin-$\frac{1}{2}$ ξ-space,

$$T(\lambda; \lambda_0, \ldots, \lambda_N) = \mathrm{Tr}_\xi\, \mathcal{T}_\xi(\lambda; \lambda_0, \ldots, \lambda_N), \tag{21.36}$$

and the monodromy matrix is the product of local Lax operators, one with index 0 for the impurity and N with indices $j = 1, \ldots, N$ for electrons:

$$\mathcal{T}_\xi(\lambda; \lambda_0, \ldots, \lambda_N) = L_{\xi N}(\lambda - \lambda_N) \cdots L_{\xi 1}(\lambda - \lambda_1) L_{\xi 0}(\lambda - \lambda_0). \tag{21.37}$$

As the generating vector of the $(2s+1)2^N$-dimensional Hilbert space, we choose the tensor product of local "up" vectors

$$\Omega = \underbrace{e^s}_{0} \otimes \underbrace{e^+}_{1} \otimes \cdots \otimes \underbrace{e^+}_{N}, \qquad e^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e^s = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{matrix} 1 \\ 2 \\ \vdots \\ 2s+1 \end{matrix}. \tag{21.38}$$

The Lax operator $L_{\xi n}$ is the identity operator at each site, except the nth site. In the case of electrons, we have

$$L_n(\lambda - \lambda_n) e_n^+ = \begin{pmatrix} a(\lambda - \lambda_n) & [\cdots] \\ 0 & b(\lambda - \lambda_n) \end{pmatrix} e_n^+, \qquad n = 1, \ldots, N. \tag{21.39}$$

The Lax operator of the impurity can be represented in the ξ-space as

$$L_0(\lambda - \lambda_0) = \begin{pmatrix} \alpha_0(\lambda - \lambda_0) & \beta_0(\lambda - \lambda_0) \\ \gamma_0(\lambda - \lambda_0) & \delta_0(\lambda - \lambda_0) \end{pmatrix}, \tag{21.40}$$

where

$$\begin{aligned} \alpha_0(\lambda - \lambda_0) &= w_0'(\lambda - \lambda_0)\mathbf{I}_0 + 2w'(\lambda - \lambda_0)\mathbf{S}_0^3, \\ \beta_0(\lambda - \lambda_0) &= 2w'(\lambda - \lambda_0)\mathbf{S}_0^-, \\ \gamma_0(\lambda - \lambda_0) &= 2w'(\lambda - \lambda_0)\mathbf{S}_0^+, \\ \delta_0(\lambda - \lambda_0) &= w_0'(\lambda - \lambda_0)\mathbf{I}_0 - 2w'(\lambda - \lambda_0)\mathbf{S}_0^3. \end{aligned} \tag{21.41}$$

The relevant operators α_0, γ_0 and δ_0 act on the highest eigenvector of spin $\mathbf{S}_0^3$ as follows

$$\begin{aligned} \alpha_0(\lambda - \lambda_0)e_0^s &= \left[\left(s + \tfrac{1}{2}\right) a'(\lambda - \lambda_0) - \left(s - \tfrac{1}{2}\right) b'(\lambda - \lambda_0)\right] e_0^s, \\ \gamma_0(\lambda - \lambda_0)e_0^s &= 0, \\ \delta_0(\lambda - \lambda_0)e_0^s &= \left[-\left(s - \tfrac{1}{2}\right) a'(\lambda - \lambda_0) + \left(s + \tfrac{1}{2}\right) b'(\lambda - \lambda_0)\right] e_0^s. \end{aligned} \tag{21.42}$$

Representing the monodromy matrix in the ξ-space as

$$\mathcal{T}(\lambda;\lambda_0,\ldots,\lambda_N)=\begin{pmatrix} A(\lambda;\lambda_0,\ldots,\lambda_N) & B(\lambda;\lambda_0,\ldots,\lambda_N)\\ C(\lambda;\lambda_0,\ldots,\lambda_N) & D(\lambda;\lambda_0,\ldots,\lambda_N)\end{pmatrix}, \tag{21.43}$$

the triangle form of Lax operators implies $C\Omega=0$, $A\Omega=t_A\Omega$ where

$$\begin{aligned} t_A(\lambda;\lambda_0,\ldots,\lambda_N) &= \left[\left(s+\frac{1}{2}\right)a'(\lambda-\lambda_0)-\left(s-\frac{1}{2}\right)b'(\lambda-\lambda_0)\right]\\ &\quad\times\prod_{n=1}^{N}a(\lambda-\lambda_n) \end{aligned} \tag{21.44}$$

and $D\Omega=t_D\Omega$ where

$$\begin{aligned} t_D(\lambda;\lambda_0,\ldots,\lambda_N) &= \left[-\left(s-\frac{1}{2}\right)a'(\lambda-\lambda_0)+\left(s+\frac{1}{2}\right)b'(\lambda-\lambda_0)\right]\\ &\quad\times\prod_{n=1}^{N}b(\lambda-\lambda_n). \end{aligned} \tag{21.45}$$

Introducing $R_{\xi\eta}(\lambda)=\mathcal{P}S_{\xi\eta}(\lambda)$ for the electron-electron scattering matrix (21.27) in the tensor product of auxiliary spin-$\frac{1}{2}$ ξ and η spaces, the YBE for the monodromy matrix reads

$$\begin{aligned} &R(\lambda-\mu)\left[\mathcal{T}(\lambda;\lambda_0,\ldots,\lambda_N)\otimes\mathcal{T}(\mu;\lambda_0,\ldots,\lambda_N)\right]\\ &=\left[\mathcal{T}(\mu;\lambda_0,\ldots,\lambda_N)\otimes\mathcal{T}(\lambda;\lambda_0,\ldots,\lambda_N)\right]R(\lambda-\mu). \end{aligned} \tag{21.46}$$

This equation implies the "homogeneous" commutation rules (8.34)-(8.36) for the operators A, B, C and D. In the spirit of the QISM, we search the eigenvectors of the transfer matrix $T=A+D$, in the subspace with $N-M$ electrons with spin up and M electrons with spin down ($M\leq N/2$), in the ansatz form

$$\psi(\lambda_0,\ldots,\lambda_N;\Lambda_1,\ldots,\Lambda_M)=\prod_{\alpha=1}^{M}B(\Lambda_\alpha;\lambda_0,\ldots,\lambda_N)\Omega, \tag{21.47}$$

where the Λ-parameters are as-yet free. Commuting the operators A and D with all B's in the eigenvalue equation $T\psi=t\psi$ lead to the eigenvalues

$$\begin{aligned} t(\lambda;\lambda_0,\ldots,\lambda_N;\Lambda_1,\ldots,\Lambda_M) &= t_A(\lambda;\lambda_0,\ldots,\lambda_N)\prod_{\alpha=1}^{M}\frac{a(\Lambda_\alpha-\lambda)}{b(\Lambda_\alpha-\lambda)}\\ &\quad+t_D(\lambda;\lambda_0,\ldots,\lambda_N)\prod_{\alpha=1}^{M}\frac{a(\lambda-\Lambda_\alpha)}{b(\lambda-\Lambda_\alpha)}. \end{aligned} \tag{21.48}$$

"Unwanted" terms, generated during the commutation procedure, are removed if Λ's satisfy the system of M coupled equations

$$t_A(\Lambda_\alpha;\lambda_0,\ldots,\lambda_N)\prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M}\frac{a(\Lambda_\beta-\Lambda_\alpha)}{b(\Lambda_\beta-\Lambda_\alpha)}$$

$$= t_D(\Lambda_\alpha;\lambda_0,\dots,\lambda_N)\prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M}\frac{a(\Lambda_\alpha-\Lambda_\beta)}{b(\Lambda_\alpha-\Lambda_\beta)},\qquad \alpha=1,\dots,M. \tag{21.49}$$

Using the relations (21.33), this system is equivalent to

$$\frac{\Lambda_\alpha-\lambda_0-\mathrm{i}g\left(s+\frac{1}{2}\right)}{\Lambda_\alpha-\lambda_0+\mathrm{i}g\left(s-\frac{1}{2}\right)}\prod_{n=1}^{N}\left(\frac{\Lambda_\alpha-\lambda_n-\mathrm{i}g}{\Lambda_\alpha-\lambda_n}\right)=\prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M}\left(\frac{\Lambda_\alpha-\Lambda_\beta-\mathrm{i}g}{\Lambda_\alpha-\Lambda_\beta+\mathrm{i}g}\right). \tag{21.50}$$

Substituting here the values of spectral parameters for the impurity and electrons (21.24) and using the substitution $\Lambda_\alpha\to g\Lambda_\alpha+\mathrm{i}g/2$, we end up with the Bethe equations for the rapidities $\{\Lambda_\alpha\}$ of the spin density waves:

$$\left(\frac{\Lambda_\alpha+i/2}{\Lambda_\alpha-i/2}\right)^N\frac{\Lambda_\alpha+1/g+\mathrm{i}s}{\Lambda_\alpha+1/g-\mathrm{i}s}=-\prod_{\beta=1}^{M}\left(\frac{\Lambda_\alpha-\Lambda_\beta+\mathrm{i}}{\Lambda_\alpha-\Lambda_\beta-\mathrm{i}}\right)\qquad \alpha=1,\dots,M. \tag{21.51}$$

The system of N eigenvalue equations (21.34) for the momenta $\{k_j\}$ of the charge density waves implies

$$\exp(\mathrm{i}k_jL)=\exp(\mathrm{i}Js/2)\prod_{\alpha=1}^{M}\frac{\Lambda_\alpha+i/2}{\Lambda_\alpha-i/2},\qquad j=1,\dots,N. \tag{21.52}$$

Note that the charge and spin sectors in the model decouple completely. The energy is given by

$$E=\sum_{j=1}^{N}k_j. \tag{21.53}$$

As the generating vector Ω has $S^z_\Omega=N/2+s$ and each of M B-operators decrease S^z_Ω by one, the total z-spin projection is

$$S^z=N/2-M+s. \tag{21.54}$$

Eqs. (21.51)-(21.54) for the impurity spin $s=\frac{1}{2}$ were obtained in Refs. [20, 21], for arbitrary spin s in Refs. [22, 23].

Taking the logarithm of Eqs. (21.51) and (21.52) results in

$$k_jL=2\pi N_j-\sum_{\alpha=1}^{M}[\theta(2\Lambda_\alpha)+\pi]-\delta_{\mathrm{ch}}(k_j), \tag{21.55}$$

$$N\theta(2\Lambda_\alpha)=2\pi J_\alpha+\sum_{\beta=1}^{M}\theta(\Lambda_\alpha-\Lambda_\beta)-\delta_{\mathrm{sp}}(\Lambda_\alpha), \tag{21.56}$$

where $\theta(\Lambda)=2\arctan\Lambda$ is the two-particle scattering phase of the spin density waves, N_j (integer for even N) and J_α (integer if M is odd and half odd integer if M is even) are quantum numbers of the system and

$$\delta_{\mathrm{ch}}(k)=-\frac{1}{2}Js,\qquad \delta_{\mathrm{sp}}(\Lambda)=\theta\left((\Lambda+g^{-1})/s\right) \tag{21.57}$$

are respectively the one-electron charge and spin phases of the scattering by the impurity. With respect to the Bethe Eqs. (21.55) and (21.56), the energy (21.53) can be expressed as

$$E = E_{\rm h}^{\rm ch} + E^{\rm sp}, \qquad E^{\rm sp} = E_{\rm h}^{\rm sp} + \frac{1}{L}E_{\rm i}, \tag{21.58}$$

where

$$E_{\rm h}^{\rm ch} = \frac{2\pi}{L}\sum_{j=1}^{N} N_j, \qquad E_{\rm h}^{\rm sp} = -\frac{2\pi}{L}\sum_{\alpha=1}^{M} J_\alpha - \frac{\pi NM}{L} \tag{21.59}$$

are the charge and spin parts of the host metal energy in the absence of the impurity and

$$E_{\rm i} = -\sum_{j=1}^{N}\delta_{\rm ch}(k_j) + \sum_{\alpha=1}^{M}\delta_{\rm sp}(\Lambda_\alpha) = \frac{1}{2}JsN + \sum_{\alpha=1}^{M}\delta_{\rm sp}(\Lambda_\alpha) \tag{21.60}$$

is the energy contribution of the impurity. Note that the energy contribution due to the impurity depends only on the spin subsystem.

21.4 Ground state

For fixed large values of N and M, first we have to determine the configuration of *distinct* quantum numbers $\{N_j\}$ and $\{J_\alpha\}$ which correspond to the ground state. In view of the above energy analysis, in the thermodynamic limit this configuration is determined exclusively by the host system of free fermions, and not by the impurity state.

- Since the integers $\{N_j\}$ in the charge energy of particles $E_{\rm h}^{\rm ch}$ (21.59) can take arbitrarily large negative values, the charge energy spectrum is unbounded from below. This unboundedness of the spectrum does not affect the impurity. Following the idea of the Fermi cut-off of momenta, we assume that each of charge energies $2\pi N_j/L$ does not exceed the Fermi energy $\varepsilon_{\rm F} = \pi N/L$, i.e. $|N_j| \le N/2$. Thus N_j are successive N integers ranging from $-N/2$ to $N/2$ and we have $E_{\rm h}^{\rm ch} = 0$ in the ground state.

- It can be shown from Eq. (21.56) that the numbers $\{J_\alpha\}$ are bounded by $-(N-M)/2 \le J_\alpha \le (N-M)/2$; the boundaries $\pm(N-M)/2$ correspond to $\Lambda \to \pm\infty$. The host spin energy $E_{\rm h}^{\rm sp}$ (21.59) attains its minimum if the J_α-sequence starts from the maximum $J_{\max} = (N-M)/2$ and goes down by unit step:

$$J_\alpha = \frac{N-M}{2} - (\alpha - 1), \qquad \alpha = 1, \ldots, M. \tag{21.61}$$

  The corresponding host spin part of the ground-state energy is

$$\begin{aligned} E_{\rm h}^{\rm sp} &= -\frac{2\pi}{L}\left[\sum_{\alpha=1}^{M}\left(\frac{N-M}{2} - (\alpha-1)\right) + \frac{MN}{2}\right] \\ &= -\frac{2\pi}{L}\left(MN - M^2 + \frac{1}{2}M\right) \sim -\frac{\pi N^2}{2L} + \frac{2\pi (S^z)^2}{L}. \end{aligned} \tag{21.62}$$

The Λ_α solutions of Eq. (21.56) are real monotonous functions of J_α numbers. Thus Λ's are distributed between the maximal $\Lambda = \infty$ and minimal $\Lambda = -Q$ values. The minimal value corresponds to the lowest $J_M = (N - 3M)/2$. The absolute ground state with $M = N/2$ ($S^z = 0$) is identified with $J_M = -N/4$, i.e. $Q = \infty$.

In the thermodynamic limit of the ground state, Λ's are distributed continuously between $-Q$ and ∞, with the density $\sigma(\Lambda)$; $\sigma(\Lambda) = 0$ for $\Lambda < -Q$. The state density $f(\Lambda) = J(\Lambda)/N$ is related to $\sigma(\Lambda)$ via $f'(\Lambda) = \sigma(\Lambda)$. The continualization of the Bethe equations (21.56) results in

$$\theta(2\Lambda) = 2\pi f(\Lambda) + \int_{-Q}^{\infty} \mathrm{d}\Lambda'\, \theta(\Lambda - \Lambda')\sigma(\Lambda') - \frac{1}{N}\delta_{\mathrm{sp}}(\Lambda). \tag{21.63}$$

The differentiation of this equation with respect to Λ leads to

$$\sigma(\Lambda) = a_1(\Lambda) + \frac{1}{N}a_{2s}(\Lambda + 1/g) - \int_{-Q}^{\infty} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma(\Lambda'), \qquad \Lambda > -Q, \tag{21.64}$$

where

$$a_n(\Lambda) = \frac{1}{2\pi}\frac{n}{\Lambda^2 + (n^2/4)}. \tag{21.65}$$

The solution of the linear Eq. (21.64) is the sum of the host metal and impurity contributions:

$$\sigma(\Lambda) = \sigma_{\mathrm{h}}(\Lambda) + \frac{1}{N}\sigma_{\mathrm{i}}(\Lambda); \tag{21.66}$$

the host metal and impurity ground-state densities satisfy the integral equations

$$\sigma_{\mathrm{h}}(\Lambda) = a_1(\Lambda) - \int_{-Q}^{\infty} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma_{\mathrm{h}}(\Lambda'), \qquad \Lambda > -Q; \tag{21.67}$$

$$\sigma_{\mathrm{i}}(\Lambda) = a_{2s}(\Lambda + 1/g) - \int_{-Q}^{\infty} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma_{\mathrm{i}}(\Lambda'), \qquad \Lambda > -Q. \tag{21.68}$$

The spin per particle

$$\frac{1}{N}S^z = \frac{1}{2} - \int_{-Q}^{\infty} \mathrm{d}\Lambda\, \sigma(\Lambda) + \frac{s}{N} \tag{21.69}$$

can also be decomposed onto the host metal and impurity parts:

$$\frac{1}{N}S^z_{\mathrm{h}} = \frac{1}{2} - \int_{-Q}^{\infty} \mathrm{d}\Lambda\, \sigma_{\mathrm{h}}(\Lambda), \qquad M_{\mathrm{i}} = s - \int_{-Q}^{\infty} \mathrm{d}\Lambda\, \sigma_{\mathrm{i}}(\Lambda). \tag{21.70}$$

Instead of considering the (local) ground state in the sector with the fixed magnetization of electrons, we prefer to apply the magnetic field H to the whole system and look for the absolute ground state in the presence of this field.

21.4.1 Zero magnetic field

If the external field $H = 0$, we have the ground state with $M = N/2$ and $Q = \infty$. The integral Eqs. (21.67) and (21.68) can be solved explicitly by the Fourier method. Using that $\hat{a}_n(\omega) = \mathrm{e}^{-n|\omega|/2}$ we obtain the following Fourier transforms of the host and impurity densities

$$\hat{\sigma}_{\mathrm{h}}(\omega) = \frac{\mathrm{e}^{-|\omega|/2}}{1+\mathrm{e}^{-|\omega|}}, \qquad \hat{\sigma}_{\mathrm{i}}(\omega) = \frac{\mathrm{e}^{-s|\omega|}}{1+\mathrm{e}^{-|\omega|}}\mathrm{e}^{-\mathrm{i}\omega/g}. \tag{21.71}$$

Inserting these results into (21.70) with $Q = \infty$ leads to

$$\frac{1}{N}S^z_{\mathrm{h}} = 0, \qquad M_{\mathrm{i}} = s - \frac{1}{2}. \tag{21.72}$$

The fact that the magnetization per electron $S^z_{\mathrm{h}}/N = 0$ was expected. The $2s$-fold degenerate ground state of the impurity means that the conduction electrons do not quench the impurity spin s completely, they are only able to decrease the impurity spin by $1/2$. The only exception is the case $s = \frac{1}{2}$ when the impurity spin is fully compensated and the impurity ground state is a singlet state.

21.4.2 Arbitrary magnetic field

In the leading order with respect to $1/N$, the magnetism of non-interacting electrons is determined by the minimization of the ground state energy (21.62) plus the magnetic field term $-HS^z$, giving

$$\frac{1}{N}S^z_{\mathrm{h}} = \frac{H}{4\varepsilon_{\mathrm{F}}}, \qquad \frac{1}{N}E^{\mathrm{sp}}_{\mathrm{h}} \sim -\frac{\varepsilon_{\mathrm{F}}}{2} - \frac{H^2}{8\varepsilon_{\mathrm{F}}}. \tag{21.73}$$

To obtain the explicit dependence of the impurity magnetization M_{i} on H, we introduce the hole ground-state density $\tilde{\sigma}(\Lambda)$. It is defined by an extension of the differential Eq. (21.64) for the particle density $\sigma(\Lambda)$ to the "forbidden" region $\Lambda < -Q$:

$$\tilde{\sigma}(\Lambda) = a_1(\Lambda) + \frac{1}{N}a_{2s}(\Lambda + 1/g) - \int_{-Q}^{\infty} \mathrm{d}\Lambda'\, a_2(\Lambda - \Lambda')\sigma(\Lambda'), \qquad \Lambda < -Q; \tag{21.74}$$

$\tilde{\sigma}(\Lambda) = 0$ for $\Lambda > -Q$. To have the Fermi point $-Q$ as the zero reference, we shift the particle and hole densities as follows

$$r(\Lambda) \equiv \sigma(\Lambda - Q), \qquad \tilde{r}(\Lambda) \equiv \tilde{\sigma}(\Lambda - Q), \tag{21.75}$$

so that $r(\Lambda) = 0$ for $\Lambda < 0$ and $\tilde{r}(\Lambda) = 0$ for $\Lambda > 0$. Let

$$\rho^+(\omega) = \int_0^{\infty} \mathrm{d}\Lambda\, \exp(\mathrm{i}\omega\Lambda) r(\Lambda), \qquad \rho^-(\omega) = \int_{-\infty}^{0} \mathrm{d}\Lambda\, \exp(\mathrm{i}\omega\Lambda)\tilde{r}(\Lambda). \tag{21.76}$$

Performing the Fourier transformation of the sum of Λ-shifted Eqs. (21.64) and (21.74), we find

$$\rho^-(\omega) + \left(1+\mathrm{e}^{-|\omega|}\right)\rho^+(\omega) = \mathrm{e}^{\mathrm{i}\omega Q}\left(\mathrm{e}^{-|\omega|/2} + \frac{1}{N}\mathrm{e}^{-s|\omega|-\mathrm{i}\omega/g}\right) \tag{21.77}$$

We divide this equation by $[1+\exp(-|\omega|)]$ and return to the original Λ space, to obtain, in the purely hole format, integral equations for the host metal and impurity hole densities

$$\tilde{r}_{\rm h}(\Lambda)+\int_{-\infty}^{0}{\rm d}\Lambda'\,J(\Lambda-\Lambda')\tilde{r}_{\rm h}(\Lambda') = \frac{1}{2\cosh\pi(\Lambda-Q)}, \qquad \Lambda<0, \tag{21.78}$$

$$\tilde{r}_{\rm i}(\Lambda)+\int_{-\infty}^{0}{\rm d}\Lambda'\,J(\Lambda-\Lambda')\tilde{r}_{\rm i}(\Lambda') = \mathcal{S}_{2s}(\Lambda-Q+1/g), \qquad \Lambda<0, \tag{21.79}$$

where

$$\begin{aligned} J(\Lambda) &= -\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{2\pi}\frac{1}{1+\exp(|\omega|)}{\rm e}^{-{\rm i}\omega\Lambda}, \\ \mathcal{S}_{2s}(\Lambda) &= \int_{-\infty}^{\infty}\frac{{\rm d}\omega}{2\pi}\frac{\exp(-s|\omega|)}{1+\exp(-|\omega|)}{\rm e}^{-{\rm i}\omega\Lambda}. \end{aligned} \tag{21.80}$$

Analogously, taking into account the relation (21.73), the spin per particle

$$\frac{1}{N}S^z=\frac{1}{2}-\rho^{+}(0)+\frac{s}{N} \tag{21.81}$$

can be decomposed in the hole format onto the following host metal and impurity parts

$$\frac{H}{2\varepsilon_{\rm F}}=\int_{-\infty}^{0}{\rm d}\Lambda\,\tilde{r}_{\rm h}(\Lambda), \qquad M_{\rm i}=s-\frac{1}{2}+\frac{1}{2}\int_{-\infty}^{0}{\rm d}\Lambda\,\tilde{r}_{\rm i}(\Lambda). \tag{21.82}$$

For the impurity with the spin $s=\frac{1}{2}$, we can derive the the impurity magnetic susceptibility at $H=0$ without knowing the explicit forms of Λ-densities. In the limit $H\to 0$ ($Q\to\infty$), we should consider only the leading terms

$$\frac{1}{2\cosh\pi(\Lambda-Q)}\sim{\rm e}^{-\pi Q+\pi\Lambda}, \qquad \mathcal{S}_1(\Lambda-Q+1/g)\sim{\rm e}^{-\pi Q+\pi\Lambda+\pi/g} \tag{21.83}$$

on the rhs of the integral Eqs. (21.78) and (21.79). The host metal and impurity hole distributions $\tilde{r}_{\rm h}(\Lambda)$ and $\tilde{r}_{\rm i}(\Lambda)$ thus differ from one another only by the factor $\exp(\pi/g)$ and we have

$$M_i=\frac{H}{4\varepsilon_{\rm F}}\exp\left(\frac{\pi}{g}\right). \tag{21.84}$$

Defining the Kondo temperature

$$T_{\rm K}=\frac{2\varepsilon_{\rm F}}{\pi}\exp\left(-\frac{\pi}{g}\right), \tag{21.85}$$

which is assumed to be finite, the magnetic susceptibility of the spin-$\frac{1}{2}$ impurity at zero temperature is given by

$$\chi_{\rm i}=\frac{\partial M_{\rm i}}{\partial H}\Big|_{H=0}=\frac{1}{2\pi T_{\rm K}}. \tag{21.86}$$

For the impurity with an arbitrary spin s, we study the regime in which the magnetic field is small comparing the Fermi energy scale, $H\ll\varepsilon_{\rm F}$. This condition means that $S^z/N\ll 1$ and

$Q \gg 1$. It is therefore sufficient to solve Eq. (21.78) in the leading order of $\exp(-\pi Q)$, i.e. $\tilde{r}_{\rm h}(\Lambda) = \exp(-\pi Q)\tilde{r}^{(0)}(\Lambda)$ where $\tilde{r}^{(0)}(\Lambda)$ is the solution of the Wiener-Hopf equation

$$\tilde{r}^{(0)}(\Lambda) + \int_{-\infty}^{0} {\rm d}\Lambda'\, J(\Lambda - \Lambda')\tilde{r}^{(0)}(\Lambda') = \exp(\pi\Lambda), \qquad \Lambda < 0. \tag{21.87}$$

The relationship between H and Q is yielded by the first relation in Eq. (21.82):

$$\frac{H(Q)}{2\varepsilon_{\rm F}} = \exp(-\pi Q) \int_{-\infty}^{0} {\rm d}\Lambda\, \tilde{r}^{(0)}(\Lambda). \tag{21.88}$$

Eq. (21.87) can be solved by using the Wiener-Hopf method explained in Sect. 14; a slight modification is due to the fact that Λ's are negative. There exists a unique factorization of

$$\frac{1}{1 + \hat{J}(\omega)} \equiv 1 + \exp(-|\omega|) = F_+(\omega)F_-(\omega), \tag{21.89}$$

where $F_+(\omega)$ and $F_-(\omega)$ are analytic and nonvanishing functions in the half-planes Π_+ and Π_-, respectively. They are related by $F_+(\omega) = F_-(-\omega)$ ($\omega \in \Pi_+$). The explicit forms of $F_\pm(\omega)$ read

$$F_\pm(\omega) = \exp\left(\mp \int \frac{{\rm d}\omega'}{2\pi{\rm i}} \frac{\ln\left(1 + {\rm e}^{-|\omega'|}\right)}{\omega - \omega' \pm {\rm i}0} \right) = \frac{\sqrt{2\pi}}{\Gamma\left(\frac{1}{2} \mp {\rm i}\frac{\omega}{2\pi}\right)} f_\pm\left(\frac{\omega}{2\pi}\right), \tag{21.90}$$

where

$$f_\pm(\omega) = \left(\frac{\mp {\rm i}\omega + 0}{\rm e} \right)^{\mp {\rm i}\omega}. \tag{21.91}$$

Due to the equality $\Gamma(\frac{1}{2} + {\rm i}x)\Gamma(\frac{1}{2} - {\rm i}x) = \pi/\cosh(\pi x)$ [67], $f_\pm(\omega)$ factorize the function

$$\exp(-\pi|\omega|) = f_+(\omega)f_-(\omega). \tag{21.92}$$

$f_+(\omega)(f_-(\omega))$ is analytic in the upper (lower) half-planes and has a cut along the lower (upper) imaginary half-axis. The discontinuities of integer powers of f-functions on the imaginary half-axes are given by

$${\rm Disc}\, f_\pm^n(\omega) = \mp 2{\rm i} \exp\left(-n|\omega| \ln\left|\frac{\omega}{e}\right| \right) \sin\left(\pi n|\omega|\right). \tag{21.93}$$

The Fourier transform of the function

$$g(\Lambda) = \begin{cases} {\rm e}^{\pi\Lambda} & \text{for } \Lambda < 0, \\ 0 & \text{for } \Lambda > 0 \end{cases} \tag{21.94}$$

is $\hat{g}(\omega) = 1/({\rm i}\omega + \pi)$. The pole of $\hat{g}(\omega)$ at $\omega = {\rm i}\pi \in \Pi_+$ is removed by subtracting the residue in the combination

$$F_+(\omega)\hat{g}(\omega) = \frac{1}{{\rm i}\omega + \pi}\left[F_+(\omega) - F_+({\rm i}\pi)\right] + \frac{F_+({\rm i}\pi)}{{\rm i}\omega + \pi}. \tag{21.95}$$

Thus we have

$$\hat{\tilde{r}}^{(0)}(\omega) = \frac{F_+(\mathrm{i}\pi)F_-(\omega)}{\mathrm{i}\omega + \pi}. \tag{21.96}$$

The relation between H and Q (21.88) becomes

$$\frac{H}{2\varepsilon_{\mathrm{F}}} = \exp(-\pi Q)\left(\frac{2}{\pi \mathrm{e}}\right)^{1/2}. \tag{21.97}$$

This formula motivates us to introduce the scale

$$Q - \frac{1}{g} = \frac{1}{\pi}\ln\left(\frac{T_H}{H}\right), \qquad T_H = \left(\frac{2\pi}{\mathrm{e}}\right)^{1/2} T_{\mathrm{K}}. \tag{21.98}$$

Now we solve formally Eq. (21.79) for the impurity hole distribution $\tilde{r}_{\mathrm{i}}(\Lambda)$ by using the Wiener-Hopf technique outlined above. Substituting the new scale (21.98) into the rhs of Eq. (21.79) and using the relations obeyed by the functions $F_\pm(\omega)$ and $f_\pm(\omega)$, we have

$$\begin{aligned} \mathcal{S}_{2s}(\Lambda - Q + 1/g) &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}(\omega+\mathrm{i}0)\Lambda}\varphi(\omega), \\ \varphi(\omega) &= \frac{f_+^{2s}\left(\frac{\omega}{2\pi}\right) f_-^{2s}\left(\frac{\omega}{2\pi}\right)}{F_+(\omega)F_-(\omega)} \exp\left(-\mathrm{i}\frac{\omega}{\pi}\ln\frac{H}{T_H}\right). \end{aligned} \tag{21.99}$$

The Fourier transform of the function under consideration

$$g(\Lambda) = \begin{cases} \mathcal{S}_{2s}(\Lambda - Q + 1/g) & \text{for } \Lambda < 0, \\ 0 & \text{for } \Lambda > 0 \end{cases} \tag{21.100}$$

is

$$\begin{aligned} \hat{g}(\omega) &= \int_{-\infty}^{0} \mathrm{d}\Lambda\, \mathrm{e}^{\mathrm{i}\omega\Lambda} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \mathrm{e}^{-\mathrm{i}(\omega'+\mathrm{i}0)\Lambda}\varphi(\omega'), \\ &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi}\varphi(\omega')\frac{1}{\mathrm{i}(\omega - \omega' - \mathrm{i}0)}. \end{aligned} \tag{21.101}$$

The poles of $\hat{g}(\omega)$ at $\omega = \omega' + \mathrm{i}0 \in \Pi_+$ are removed by subtracting the residues in the combination $F_+(\omega)\hat{g}(\omega)$. Consequently,

$$\hat{\tilde{r}}_{\mathrm{i}}(\omega) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi}\varphi(\omega')\frac{F_+(\omega' + \mathrm{i}0)F_-(\omega)}{\mathrm{i}(\omega - \omega' - \mathrm{i}0)}. \tag{21.102}$$

From the integral representation of the impurity magnetization M_{i} at $T = 0$ (21.82) we finally obtain

$$\begin{aligned} M_{\mathrm{i}} &= s - \frac{1}{2} + \frac{1}{2}\hat{\tilde{r}}_{\mathrm{i}}(0) \\ &= s - \frac{1}{2} + \frac{\mathrm{i}}{4\pi^{3/2}} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\Gamma\left(\frac{1}{2} + \mathrm{i}\omega\right)}{\omega + \mathrm{i}0} f_+^{2s}(\omega) f_-^{2s-1}(\omega) \mathrm{e}^{-2\mathrm{i}\omega\ln(H/T_H)}. \end{aligned} \tag{21.103}$$

We see that the impurity magnetization is the universal function of H/T_H. In dependence on the value of the ratio H/T_H, it has two different series representations.

If $H > T_H$, the contour of integration envelops the lower half-plane Π_-. There is one pole at $\omega = -\mathrm{i}0$ and the branch cut of $f_+(\omega)$ across the negative part of the imaginary axis, so that

$$M_{\mathrm{i}}(H > T_H) \quad = \quad s - \frac{1}{2\pi^{3/2}} \int_0^\infty \mathrm{d}\omega \, \frac{\Gamma\left(\frac{1}{2}+\omega\right)}{\omega} \sin(2\pi s\omega) \times \left(\frac{\omega}{\mathrm{e}}\right)^{-\omega} \mathrm{e}^{-2\omega \ln(H/T_H)}. \tag{21.104}$$

We introduce the "invariant charge" $z(H/T_H) > 0$ which satisfies the Gell-Mann-Low equation [25, 26]

$$\frac{1}{z} - \frac{1}{2} \ln z = \ln\left(\frac{H}{T_H}\right), \quad z = \frac{1}{\ln(H/T_H)} + \frac{1}{2\ln^2(H/T_H)} \ln\left[\ln(H/T_H)\right] + \cdots. \tag{21.105}$$

Thus the formula (21.104) can be rewritten as

$$M_{\mathrm{i}}(H > T_H) = s - \frac{1}{2\pi^{3/2}} \int_0^\infty \mathrm{d}t \, \frac{\Gamma\left(\frac{1}{2}+zt\right)}{t} \sin(2\pi szt) \left(\frac{t}{\mathrm{e}}\right)^{-zt} \mathrm{e}^{-2t}. \tag{21.106}$$

The consequent expansion in powers of z results in

$$M_{\mathrm{i}}(H > T_H) = s\left(1 + \sum_{n=1}^\infty \alpha_n(s) z^n\right). \tag{21.107}$$

This expansion is asymptotic.

If $H < T_H$, the integration contour envelops the upper half-plane Π_+. The contour can be deformed to encircle the positive part of the imaginary axis where only singularities of the integrand are situated. The analysis of the integral in (21.103) then depends on whether the impurity spin $s = \frac{1}{2}$ or $s > \frac{1}{2}$.

In the $s = \frac{1}{2}$ case, the only singularities are the simple poles of the Γ function at the points $\omega = \mathrm{i}(n + 1/2)$ $(n = 0, 1, \ldots)$ and we have

$$M_{\mathrm{i}}^{(1/2)}(H < T_H) = \frac{1}{2\sqrt{\pi}} \sum_{n=0}^\infty \frac{(-1)^n}{n!(n+1/2)} \left(\frac{n+1/2}{\mathrm{e}}\right)^{n+1/2} \left(\frac{H}{T_H}\right)^{2n+1}. \tag{21.108}$$

This expansion is absolutely convergent.

In the $s > \frac{1}{2}$ case, the cut of $f_-(\omega)$ across the positive part of the imaginary axis is relevant and the poles of the Γ function give only exponentially small corrections. In terms of the invariant charge $z(H/T_H) < 0$, now defined by

$$\frac{1}{z} - \frac{1}{2} \ln|z| = \ln\left(\frac{H}{T_H}\right), \tag{21.109}$$

we obtain

$$M_{\mathrm{i}}^{(s)}(H < T_H) = \left(s - \frac{1}{2}\right)\left(1 + \sum_{n=1}^\infty \alpha_n(s-1/2) z^n\right) + O\left(\frac{\exp(-1/|z|)}{\sqrt{|z|}}\right), \tag{21.110}$$

where the coefficients $\{\alpha_n\}$ are the same functions of their arguments like in the high magnetic-field series (21.107). This duality of the low and high magnetic-field series has a counterpart also for $T > 0$: We shall show later that the temperature dependence of the thermodynamic quantities for the impurity is dual in the cases $T > T_{\rm K}$ and $T < T_{\rm K}$.

21.5 Thermodynamics with strings

For $T \neq 0$, we have to consider all possible solutions for spin rapidities in the Bethe ansatz Eqs. (21.51). These equations resemble those derived for the isotropic XXX Heisenberg ring; without saying it, we shall often adopt techniques and the notation from Sect. 16.

For a large system, spin rapidity solutions form M_n strings of lengths $n = 1, 2, \ldots$, constrained by $\sum_{n=1}^{\infty} nM_n = M$. Strings of order n are characterized by M_n different real centers Λ_α^n $(\alpha = 1, \ldots, M_n)$. The string corresponds to the set of spin rapidities with equidistant imaginary parts,

$$\Lambda_\alpha^{(n,r)} = \Lambda_\alpha^n + {\rm i}\left(\frac{n+1}{2} - r\right), \qquad r = 1, \ldots, n. \tag{21.111}$$

The Bethe Eqs. (21.51) can be transformed to the ones containing only the real string centers:

$$[e_n(\Lambda_\alpha^n)]^N \, e_{n,2s}(\Lambda_\alpha^n + 1/g) = (-1)^n \prod_{m=1}^{\infty} \prod_{\beta=1}^{M_m} E_{nm}(\Lambda_\alpha^n - \Lambda_\beta^m), \tag{21.112}$$

where

$$e_{n,2s}(\Lambda) = \prod_{r=1}^{n} \frac{\Lambda + {\rm i}\left(\frac{n+1}{2} - r + s\right)}{\Lambda + {\rm i}\left(\frac{n+1}{2} - r - s\right)}. \tag{21.113}$$

In the format of string centers, the Bethe equations for electron momenta (21.52) take the form

$$\exp({\rm i}k_j L) = \exp({\rm i}Js/2) \prod_{n=1}^{\infty} \prod_{\alpha=1}^{M_n} e_n(\Lambda_\alpha^n). \tag{21.114}$$

Taking the logarithm of this and previous equations, we obtain

$$k_j L = 2\pi N_j - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} [\theta_n(\Lambda_\alpha^n) + \pi] - \delta_{\rm ch}(k) \tag{21.115}$$

and

$$N\theta_n(\Lambda_\alpha^n) = 2\pi J_\alpha^n + \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_n} \Theta_{nm}(\Lambda_\alpha^n - \Lambda_\beta^m) - \delta_{n,2s}(\Lambda_\alpha^n + 1/g), \tag{21.116}$$

where the one-electron charge and string phases of the scattering by the impurity are given by

$$\delta_{\rm ch}(k) = -\frac{Js}{2}, \qquad \delta_{n,2s}(\Lambda) = \sum_{r=1}^{\min(n,2s)} \theta_{n+2s+1-2r}(\Lambda). \tag{21.117}$$

The quantum (integer or half odd integer) numbers J_α^n are constrained by the inequality $|J_\alpha^n| \leq [N + M_n + \min(n, 2s) - 1]/2 + n - \sum_{m=1}^{\infty} \min(n, m) M_m$.

In the thermodynamic limit $N \to \infty$, one may introduce density distributions of n-string particle and hole centers $\sigma_n(\Lambda)$ and $\tilde{\sigma}_n(\Lambda)$, respectively. From Eq. (21.116) we obtain the counting function

$$h^n(\Lambda) = \frac{1}{2\pi} \left[\theta_n(\Lambda) + \frac{1}{N} \delta_{n,2s}(\Lambda + 1/g) - \frac{1}{N} \sum_{m=1}^{\infty} \sum_{\beta=1}^{M_m} \Theta_{nm}(\Lambda - \Lambda_\beta^m) \right]. \tag{21.118}$$

It determines the constraint between the n-string particle and hole densities via

$$\sigma_n(\Lambda) + \tilde{\sigma}_n(\Lambda) = \frac{\mathrm{d}h^n}{\mathrm{d}\Lambda}. \tag{21.119}$$

This set of constraints can be expressed in the matrix form as

$$\tilde{\sigma}_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\Lambda) = a_n(\Lambda) + \frac{1}{N} a_{n,2s}(\Lambda + 1/g), \tag{21.120}$$

where

$$a_{n,2s}(\Lambda) = \sum_{r=1}^{\min(n,2s)} a_{n+2s+1-2r}(\Lambda) = A_{n,2s} * s(\Lambda). \tag{21.121}$$

The spin per particle is

$$\frac{1}{N} S^z = \frac{1}{2} - \sum_{n=1}^{\infty} n \int \mathrm{d}\Lambda \, \sigma_n(\Lambda). \tag{21.122}$$

According to Eq. (21.115), the energy of the system in the presence of the magnetic field $E = \sum_{j=1}^{N} k_j - HS^z$ is given by $E = E_{\mathrm{h}}^{\mathrm{ch}} + E^{\mathrm{sp}} - HS^z$, where

$$E_{\mathrm{h}}^{\mathrm{ch}} = \frac{2\pi}{L} \sum_{j=1}^{N} N_j, \qquad \frac{1}{N} E^{\mathrm{sp}} = -\frac{N}{L} \sum_{n=1}^{\infty} \int \mathrm{d}\Lambda \, \sigma_n(\Lambda) \left[\theta_n(\Lambda) + \pi \right]. \tag{21.123}$$

The free energy at temperature T, $F = E - TS$ with S being the entropy defined by (16.33), is the functional of n-string particle densities $\{\sigma_n(\Lambda)\}$ and hole densities $\{\tilde{\sigma}_n(\Lambda)\}$. The equilibrium state is determined by the variational condition $\delta F = 0$, under the constraints $\delta\tilde{\sigma}_n = -\sum_{m=1}^{\infty} A_{nm} * \delta\sigma_m$ implied by Eq. (21.120). For excitation energies of n-strings at a given T, defined by

$$\epsilon_n(\Lambda) = T \ln \frac{\tilde{\sigma}_n^{\mathrm{eq}}(\Lambda)}{\sigma_n^{\mathrm{eq}}(\Lambda)} \qquad n = 1, 2, \ldots, \tag{21.124}$$

we obtain an infinite TBA chain of coupled non-linear integral equations:

$$\begin{aligned} T \ln[1 + \exp(\epsilon_n/T)] &= T \sum_{m=1}^{\infty} A_{nm} * \ln[1 + \exp(-\epsilon_m/T)] \\ &\quad + Hn - \frac{\varepsilon_{\mathrm{F}}}{\pi}(\theta_n + \pi). \end{aligned} \tag{21.125}$$

Applying the inverse matrix A^{-1}, we obtain another form of these equations

$$\epsilon_n(\Lambda) = Ts * \ln[1+\exp(\epsilon_{n-1}(\Lambda)/T)]\ln[1+\exp(\epsilon_{n+1}(\Lambda)/T)] - \frac{2\varepsilon_{\rm F}}{\pi}\arctan\left[\exp(\pi\Lambda)\right]\delta_{n1}, \qquad \lim_{n\to\infty}\frac{\epsilon_n}{n} = H. \tag{21.126}$$

The spin part of the free energy reads

$$\frac{1}{N}F^{\rm sp} = \sum_{n=1}^{\infty}\int {\rm d}\Lambda\left\{\sigma_n\left[Hn - \frac{\varepsilon_{\rm F}}{\pi}(\theta_n+\pi) - T\ln[1+\exp(\epsilon_n/T)]\right] + \tilde{\sigma}_n T\ln[1+\exp(-\epsilon_n/T)]\right\} - H\left(\frac{1}{2}+\frac{s}{N}\right). \tag{21.127}$$

Eliminating $\tilde{\sigma}_n$ by using Eq. (21.120), the coefficient of σ_n vanishes by virtue of the TBA equations (21.125) and we find

$$\frac{1}{N}F^{\rm sp} = -T\sum_{n=1}^{\infty}\int {\rm d}\Lambda\ \left[a_n(\Lambda) + \frac{1}{N}a_{n,2s}(\Lambda+1/g)\right] \times \ln\left(1+\exp[-\epsilon_n(\Lambda)/T]\right) - H\left(\frac{1}{2}+\frac{s}{N}\right). \tag{21.128}$$

This formula can be further simplified. Let us consider the $n=1$ case of Eq. (21.125)

$$T\ln[1+\exp(\epsilon_1/T)] = T\sum_{m=1}^{\infty}(a_{m-1}+a_{m+1}) * \ln[1+\exp(-\epsilon_m/T)] + H - \frac{\varepsilon_{\rm F}}{\pi}(\theta_1+\pi). \tag{21.129}$$

Applying on this equation $\int_{-\infty}^{\infty}{\rm d}\Lambda\, s(\Lambda)$ and using the relation $\hat{s}(\omega)[\hat{a}_{n-1}(\omega)+\hat{a}_{n+1}(\omega)] = \hat{a}_n(\omega)$, we obtain

$$T\sum_{n=1}^{\infty}\int {\rm d}\Lambda\, a_n(\Lambda)\ln\left(1+\exp[-\epsilon_n(\Lambda)/T]\right) + \frac{H}{2} = T\int {\rm d}\Lambda\, s(\Lambda)\ln\left(1+\exp[\epsilon_1(\Lambda)/T]\right) + \frac{\varepsilon_{\rm F}}{2}. \tag{21.130}$$

Similarly, considering the $n=2s$ case of Eq. (21.125), applying on this equation the operation $\int_{-\infty}^{\infty}{\rm d}\Lambda\, s(\Lambda+1/g)$ and using the equality (21.121), we arrive at

$$T\sum_{n=1}^{\infty}\int {\rm d}\Lambda\, a_{n,2s}(\Lambda+1/g)\ln\left(1+\exp[-\epsilon_n(\Lambda)/T]\right) + Hs = T\int {\rm d}\Lambda\, s(\Lambda+1/g)\ln\left(1+\exp[\epsilon_{2s}(\Lambda)/T]\right) + {\rm const.} \tag{21.131}$$

Up to an irrelevant constant, the spin part of the free energy takes the form

$$\begin{aligned}\frac{1}{N}F^{\rm sp} &= -T\int {\rm d}\Lambda\, s(\Lambda)\ln\left(1+\exp[\epsilon_1(\Lambda)/T]\right)\\ &\quad -\frac{T}{N}\int {\rm d}\Lambda\, s(\Lambda+1/g)\ln\left(1+\exp[\epsilon_{2s}(\Lambda)/T]\right).\end{aligned} \tag{21.132}$$

The spectrum of the charge subsystem is bounded from below by $N_j \geq -N/2$. The thermodynamics of N non-interacting spinless fermions with linear kinetic energy is described by the partition function

$$Z^{\rm ch} \propto \sum_{\{N_j\}} \exp\left(-\frac{1}{T}\sum_{j=1}^{N}\frac{2\pi}{L}N_j\right) = \prod_{n=-N/2}^{\infty}\left[1+\exp\left(-\frac{2\pi}{TL}n\right)\right]. \tag{21.133}$$

For large $\varepsilon_{\rm F} = \pi N/L$, the corresponding charge part of the free energy per electron

$$\frac{1}{N}F_{\rm h}^{\rm ch} = -\frac{T}{2\varepsilon_{\rm F}}\int_{-\varepsilon_{\rm F}}^{\infty}{\rm d}k\,\ln\left[1+\exp(-k/T)\right] + \frac{\varepsilon_{\rm F}}{4} \sim -\frac{\pi^2}{12}\frac{T^2}{\varepsilon_{\rm F}} \tag{21.134}$$

is half the free energy of a non-interacting electron gas at $H = 0$.

21.6 TBA for non-interacting electron gas

The split of the electron system onto the charge and spin subsystems and the appearance of string excitations in the spectrum are very special features of our formalism, due to the presence of the impurity. To discuss the thermodynamics of the impurity, first we have to understand how the system of free spin-$\frac{1}{2}$ electrons is described by the present TBA equations.

In the absence of the impurity, the constraints among the particle and hole densities (21.120) take the form

$$\tilde{\sigma}_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\Lambda) = a_n(\Lambda). \tag{21.135}$$

Let TBA equations (21.125), taken at the rapidity Λ, be differentiated with respect to Λ. Comparing with Eq. (21.135) and recalling that $a_n(\Lambda) = \theta'(\Lambda)/(2\pi)$, we get

$$\sigma_n(\Lambda) = -\frac{1}{2\varepsilon_{\rm F}}\frac{\partial\epsilon_n(\Lambda)}{\partial\Lambda}n\left(\epsilon_n(\Lambda)\right), \quad \tilde{\sigma}_n(\Lambda) = -\frac{1}{2\varepsilon_{\rm F}}\frac{\partial\epsilon_n(\Lambda)}{\partial\Lambda}\left[1-n\left(\epsilon_n(\Lambda)\right)\right], \tag{21.136}$$

where $n(\epsilon) = [1+\exp(\epsilon/T)]^{-1}$ is the Fermi distribution function. Since the densities σ_n and $\tilde{\sigma}_n$ must be positive, the energies $\epsilon_n(\Lambda)$ are decreasing functions of Λ. The average number of n-strings at temperature T is given by

$$\frac{\langle M_n\rangle}{N} = \int_{-\infty}^{\infty}{\rm d}\Lambda\,\sigma_n(\Lambda) = \frac{T}{2\varepsilon_{\rm F}}\ln\left(\frac{1+\exp\left[-\epsilon_n(+\infty)/T\right]}{1+\exp\left[-\epsilon_n(-\infty)/T\right]}\right). \tag{21.137}$$

Let us now consider the spin part of the free energy in the absence of the impurity. From Eq. (21.128) we have

$$\frac{1}{N}F_{\rm h}^{\rm sp} = T\sum_{n=1}^{\infty}\int {\rm d}\Lambda\, a_n(\Lambda)\ln\left[1-n\left(\epsilon_n(\Lambda)\right)\right] - \frac{H}{2}. \tag{21.138}$$

Considering the equality $A_{nm}(\Lambda) = \delta(\Lambda)\delta_{nm} + \Theta'_{nm}(\Lambda)/(2\pi)$ in Eq. (21.125) and afterwards differentiating this equation with respect to Λ, we obtain

$$a_n(\Lambda) = -\frac{1}{2\varepsilon_{\rm F}}\frac{\partial\epsilon_n(\Lambda)}{\partial\Lambda} + \frac{T}{4\pi\epsilon_{\rm F}}\sum_{m=1}^{\infty}\Theta''_{nm} * \ln\left(1+\exp\left[-\epsilon_n(\Lambda)/T\right]\right). \tag{21.139}$$

Substituting this relation into (21.138), the second term with Θ'' gives zero contribution because Θ is an odd continuous function and we arrive at

$$\frac{1}{N}F_{\rm h}^{\rm sp} = \frac{T}{2\varepsilon_{\rm F}}\sum_{n=1}^{\infty}\int_{\min\epsilon_n}^{\max\epsilon_n}{\rm d}\epsilon\,\ln\left[1-n(\epsilon)\right] - \frac{H}{2}. \tag{21.140}$$

Since every $\epsilon_n(\Lambda)$ is a decreasing function of Λ, it holds that $\bar{\epsilon}_n \equiv \max\epsilon_n(\Lambda) = \epsilon(-\infty)$ and $\tilde{\epsilon}_n \equiv \min\epsilon_n(\Lambda) = \epsilon(\infty)$. The most convenient way to establish the two limits is to use TBA equations (21.126). For the $\max$ limit, setting $\Lambda \to -\infty$ we have the coupled set of equations

$$\bar{\epsilon}_n = -\frac{T}{2}\ln\left[n(\bar{\epsilon}_{n+1})n(\bar{\epsilon}_{n-1})\right]; \qquad \bar{\epsilon}_0 = -\infty, \quad \lim_{n\to\infty}\frac{\bar{\epsilon}_n}{n} = H. \tag{21.141}$$

The general solution of these second-order difference equations is

$$\bar{\epsilon}_n = T\ln\left(\Phi_n^2 - 1\right), \qquad \Phi_n = \frac{az^n - (az^n)^{-1}}{z - z^{-1}}. \tag{21.142}$$

The parameters a and z are determined by the $n = 0$ and $n \to \infty$ boundary conditions as follows $a = z = \exp(H/2T)$, hence

$$\Phi_n = \frac{\sinh[(H/2T)(n+1)]}{\sinh(H/2T)}. \tag{21.143}$$

For the $\min$ limit, setting $\Lambda \to \infty$ in (21.126) we have $\epsilon_1 \to -\varepsilon_{\rm F} \ll -T$. Taking $n(\epsilon_1) = 1$, we get the chain of equations for $\tilde{\epsilon}_n$:

$$\tilde{\epsilon}_n = -\frac{T}{2}\ln\left[n(\tilde{\epsilon}_{n+1})n(\tilde{\epsilon}_{n-1})\right]; \qquad n = 2,3,\ldots, \quad \lim_{n\to\infty}\frac{\tilde{\epsilon}_n}{n} = H. \tag{21.144}$$

The solution of this chain is $\tilde{\epsilon}_n = \bar{\epsilon}_{n-1} = T\ln(\Phi_{n-1}^2 - 1)$ $(n = 2,3,\ldots)$, i.e. the minimum ϵ limit for n strings coincides with the maximum ϵ limit for $n-1$ strings. For $H = 0$, the expression (21.140) thus becomes

$$\frac{1}{N}F_{\rm h}^{\rm sp} = -\frac{T}{2\varepsilon_{\rm F}}\int_{-\varepsilon_{\rm F}}^{\infty}{\rm d}\epsilon\,\ln\left[1+\exp(-\epsilon/T)\right] \sim -\frac{\varepsilon_{\rm F}}{4} - \frac{\pi^2}{12}\frac{T^2}{\varepsilon_{\rm F}}. \tag{21.145}$$

For $H \neq 0$, with regard to Eq. (21.73) we have

$$\frac{1}{N}F_{\rm h}^{\rm sp} \sim -\frac{\varepsilon_{\rm F}}{4} - \frac{\pi^2}{12}\frac{T^2}{\varepsilon_{\rm F}} - \frac{H^2}{8\varepsilon_{\rm F}}. \tag{21.146}$$

The total (charge plus spin) host free energy per electron reads

$$\frac{1}{N}F_{\rm h} \sim -\frac{\varepsilon_{\rm F}}{4} - \frac{\pi^2}{6}\frac{T^2}{\varepsilon_{\rm F}} - \frac{H^2}{8\varepsilon_{\rm F}}. \tag{21.147}$$

We see that while the magnetic susceptibilities of the host spin subsystem and the electron gas coincide, $\chi_{\rm h}^{\rm sp} = \chi_{\rm h} = 1/(4\varepsilon_{\rm F})$, the heat capacities differ from one another by the factor two, $C_{\rm h}^{\rm sp} = C_{\rm h}/2 = \pi^2 T/(6\varepsilon_{\rm F})$. Thus the following important equalities hold:

$$\frac{C_{\rm h}^{\rm sp}}{T\chi_{\rm h}^{\rm sp}} = \frac{1}{2}\frac{C_{\rm h}}{T\chi_{\rm h}} = \frac{2\pi^2}{3}. \tag{21.148}$$

Such relations are typical for Fermi liquids.

21.7 Thermodynamics of the impurity

The free energy (21.132) splits into the spin part of the host free energy $F_{\rm h}^{\rm sp}$ and the impurity free energy $F_{\rm i}$ defined as follows

$$\begin{aligned} F_{\rm h}^{\rm sp} &= -T\int_{-\infty}^{\infty} {\rm d}\Lambda\, s(\Lambda)\ln\left(1+\exp\left[\epsilon_1(\Lambda)/T\right]\right), \\ F_{\rm i} &= -T\int_{-\infty}^{\infty} {\rm d}\Lambda\, s(\Lambda+1/g)\ln\left(1+\exp\left[\epsilon_{2s}(\Lambda)/T\right]\right). \end{aligned} \tag{21.149}$$

Our task is to derive the thermodynamics of the impurity in the scaling regime $\varepsilon_{\rm F}\to\infty$, keeping the temperature, and in particular the Kondo temperature (21.85), finite.

Let us shift everywhere the spectral parameter $\Lambda \to \Lambda + (1/\pi)\ln(\pi T/2\varepsilon_{\rm F})$ and define

$$\epsilon'_n(\Lambda) \equiv \frac{1}{T}\epsilon_n\left(\Lambda + \frac{1}{\pi}\ln\frac{\pi T}{2\varepsilon_{\rm F}}\right). \tag{21.150}$$

Then the TBA equations (21.126) can be replaced by

$$\begin{aligned} \epsilon'_n(\Lambda) &= s * \ln[1+\exp(\epsilon'_{n-1}(\Lambda))][1+\exp(\epsilon'_{n+1}(\Lambda))] \\ &\quad -\frac{2\varepsilon_{\rm F}}{\pi T}\arctan\left[\frac{\pi T}{2\varepsilon_{\rm F}}\exp(\pi\Lambda)\right]\delta_{n1}, \qquad \lim_{n\to\infty}\frac{\epsilon'_n}{n} = \frac{H}{T}. \end{aligned} \tag{21.151}$$

and the free energies (21.149) are written as

$$\begin{aligned} F_{\rm h}^{\rm sp} &= -T\int_{-\infty}^{\infty} {\rm d}\Lambda\, s\left(\Lambda + \frac{1}{\pi}\ln\frac{\pi T}{2\varepsilon_{\rm F}}\right)\ln\left(1+\exp\left[\epsilon'_1(\Lambda)\right]\right), \\ F_{\rm i} &= -T\int_{-\infty}^{\infty} {\rm d}\Lambda\, s\left(\Lambda + \frac{1}{\pi}\ln\frac{T}{T_{\rm K}}\right)\ln\left(1+\exp\left[\epsilon'_{2s}(\Lambda)\right]\right). \end{aligned} \tag{21.152}$$

Since $T \ll \varepsilon_{\rm F}$, the main contribution to the integral comes from the region

$$|\Lambda| \sim \left|\frac{1}{\pi}\ln\frac{T}{T_{\rm K}}\right| \ll \frac{1}{\pi}\ln\frac{\varepsilon_{\rm F}}{T}.$$

Within this region, the inhomogeneous $n=1$ term $(2\varepsilon_{\rm F}/\pi T)\arctan[(\pi T/2\varepsilon_{\rm F})\exp(\pi\Lambda)]$ in the TBA chain (21.151) may be substituted by $\exp(\pi\Lambda)$. We introduce the dimensionless functions $\varphi_n(\Lambda) \equiv \epsilon'_n(\Lambda)|_{\varepsilon_{\rm F}\to\infty}$ which depend on H/T. They satisfy the universal set of coupled equations

$$\varphi_n(\Lambda) = s * \ln[1+\exp(\varphi_{n-1}(\Lambda))][1+\exp(\varphi_{n+1}(\Lambda))] - \exp(\pi\Lambda)\delta_{n1} \tag{21.153}$$

with the boundary conditions

$$\varphi_0(\Lambda) = -\infty, \qquad \lim_{n\to\infty} \frac{\varphi_n(\Lambda)}{n} = \frac{H}{T}. \tag{21.154}$$

It is convenient to introduce the new functions

$$C_n(\Lambda) = \ln\left(1 + \exp[\varphi_n(\Lambda)]\right) \tag{21.155}$$

for which the chain of coupled equations reads

$$C_n(\Lambda) = \ln\left\{1 + \exp\left[-\delta_{n1}\mathrm{e}^{\pi\Lambda} + s * (C_{n-1}(\Lambda) + C_{n+1}(\Lambda))\right]\right\}, \qquad C_0 = 0. \tag{21.156}$$

Then F_{i}, being a universal function of H/T and T/T_{K}, is expressible as

$$F_{\mathrm{i}} = -\frac{T}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \exp\left(-\frac{\mathrm{i}\omega}{\pi}\ln\frac{T}{T_{\mathrm{K}}}\right)\frac{\hat{C}_{2s}(\omega, H/T)}{2\cosh(\omega/2)}, \tag{21.157}$$

where $\hat{C}_n(\omega, H/T)$ is the standard Fourier transform of $C_n(\Lambda, H/T)$.

It is instructive to derive F_{i} in the limits of high ($T/T_{\mathrm{K}} \to \infty$) and low ($T/T_{\mathrm{K}} \to 0$) temperatures. With regard to the definition of the Kondo temperature (21.85), these limits correspond to the weak-coupling $g \to 0$ and strong-coupling $g \to \infty$ regimes, respectively. When $T/T_{\mathrm{K}} \to \infty$, the integral representation (21.152) implies that

$$F_{\mathrm{i}}(T \gg T_{\mathrm{K}}) \to -\frac{T}{2}\ln\left[1 + \exp(\bar{\epsilon}_{2s}/T)\right] = -T\ln\left[\frac{\sinh(H/2T)(2s+1)}{\sinh H/2T}\right]. \tag{21.158}$$

This is the result for an isolated impurity with spin s which indicates that, at high temperatures, the impurity decouples from conduction electrons. In the opposite limit $T/T_{\mathrm{K}} \to 0$, we find

$$F_{\mathrm{i}}(T \ll T_{\mathrm{K}}) \to -\frac{T}{2}\ln\left[1 + \exp(\bar{\epsilon}_{2s}/T)\right] = -T\ln\left[\frac{\sinh Hs/T}{\sinh H/2T}\right]. \tag{21.159}$$

This result is in full agreement with the $T = 0$ finding (21.72) that in the ground state the conduction electrons decrease the impurity spin s by $1/2$.

If $s = \frac{1}{2}$ and $H/T \ll 1$, the impurity part of the free energy can be expanded in powers of T/T_{K} [27]. It follows from Eqs. (21.153) that $\varphi_1(\Lambda) \to -\exp(\pi\Lambda)$ as $\Lambda \to \infty$. This means that the Fourier integral

$$\hat{C}_1(\omega, H/T) = \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \exp(-\mathrm{i}\omega\Lambda)\ln\left(1 + \exp\left[\varphi_1(\Lambda)\right]\right) \tag{21.160}$$

is finite (analytic) in the upper half-plane $\omega \in \Pi_+$. For $T \ll T_{\mathrm{K}}$, the contour of integration in (21.157) envelopes Π_+ and the integral can be evaluated via an infinite sequence of residues of $1/\cosh(\omega/2)$. The result is an expansion in powers of T/T_{K}:

$$F_{\mathrm{i}}^{1/2} = -T\sum_{n=0}^{\infty}(-1)^n\hat{C}_1(\mathrm{i}\pi(n+1/2), H/T)\left(\frac{T}{T_{\mathrm{K}}}\right)^{2n+1}. \tag{21.161}$$

To estimate $\hat{C}_1(\mathrm{i}\pi(n+1/2), H/T)$ for large n, we substitute the $\Lambda \to \infty$ asymptotic of $\varphi_1(\Lambda) \sim -\exp(\pi\Lambda)$ into (21.160) and obtain $\hat{C}_1(\mathrm{i}\pi(n+1/2), H/T) \sim n!$ for large n, i.e. the expansion

(21.161) is the asymptotic one. To determine the expansion coefficients $\hat{C}_1(\mathrm{i}\pi(n+1/2), H/T)$, we have to know the function $\varphi_1(\Lambda)$ in the whole range of Λ. The only exception is the leading $T \to 0$ coefficient $\hat{C}_1(\mathrm{i}\pi/2, H/T)$ which can be found indirectly by the following reasonings. We see from Eq. (21.152) that the expressions for the free energy of the spin subsystem and the $s = \frac{1}{2}$ impurity are similar and they coincide in the strong coupling limit $g \to \infty$. Consequently,

$$\frac{C_{\mathrm{i}}}{C_{\mathrm{h}}^{\mathrm{sp}}} = \frac{2\varepsilon_{\mathrm{F}}}{\pi T_{\mathrm{K}}}. \tag{21.162}$$

In the ground state Eq. (21.86) we found that the magnetic susceptibility $\chi_{\mathrm{i}} = 1/(2\pi T_{\mathrm{K}})$, hence

$$\frac{C_{\mathrm{i}}}{T\chi_{\mathrm{i}}} = \frac{C_{\mathrm{h}}^{\mathrm{sp}}}{T\chi_{\mathrm{h}}^{\mathrm{sp}}} = \frac{1}{2}\frac{C_{\mathrm{h}}}{T\chi_{\mathrm{h}}} = \frac{2\pi^2}{3} \tag{21.163}$$

and we arrive at

$$\hat{C}_1(\mathrm{i}\pi/2, H/T) = \frac{\pi}{6} + \frac{1}{4\pi}\left(\frac{H}{T}\right)^2. \tag{21.164}$$

The relation (21.163) is known as the Wilson-Nozières formula for a Fermi liquid.

To derive the thermodynamics of the impurity with spin $s > \frac{1}{2}$, first we have to analyze the analytic properties of the Fourier transform $\hat{C}_n(\omega, H/T)$ with $n = 2s > 1$. In the limits $\Lambda \to \pm\infty$, it holds that $\varphi_n(\Lambda) = \epsilon_n'(\Lambda) = \epsilon_n(\Lambda)/T$. The asymptotic analysis of $\epsilon_n(\Lambda \to \pm\infty)$ between Eqs. (21.138)-(21.141) tells us that

$$C_n(\Lambda) = \begin{cases} 2\ln\Phi_n & \text{for } \Lambda \to -\infty, \\ 2\ln\Phi_{n-1} & \text{for } \Lambda \to \infty. \end{cases} \tag{21.165}$$

Hence, in the neigbourhood of $\omega = 0$ the Fourier transform of $C_n(\Lambda, H/T)$ can be expressed as

$$\hat{C}_n(\omega) = 2\mathrm{i}\frac{\ln\Phi_n}{\omega + \mathrm{i}0} - 2\mathrm{i}\frac{\ln\Phi_{n-1}}{\omega - \mathrm{i}0} + \hat{D}_n(\omega), \tag{21.166}$$

where $\hat{D}_n(\omega)$ is finite at $\omega = 0$. $\hat{D}_n(\omega)$ $(n > 1)$ is expected to possess the following properties:

- $\hat{D}_n(\omega)$ has cuts along the imaginary axis, starting from $\omega = 0$, in both lower and upper half-planes.
- The discontinuities at the upper and lower cuts are dual in the sense that

$$\mathrm{Disc}\,\hat{D}_{n+1}(\mathrm{i}|\omega|) = \mathrm{Disc}\,\hat{D}_n(-\mathrm{i}|\omega|). \tag{21.167}$$

- $$\mathrm{Disc}\,\hat{D}_n(-\mathrm{i}|\omega|) = \hat{B}_n(|\omega|, T/H)\left(\frac{|\omega|}{2\pi}\right)^{-|\omega|/2\pi}, \tag{21.168}$$

  where $\hat{B}_n(\omega, T/H)$ is analytic in the whole plane except at the cuts and has zeros at $\omega = -\mathrm{i}\pi(2k+1)$ $(k = 0, 1, \ldots)$.

These properties of $\hat{C}_n(\omega)$, which will be checked in special cases, allow us to perform a general analysis of the free energy of the spin-s impurity by using the relation (21.157).

If $T > T_{\rm K}$, closing the integration contour in the lower half-plane, the cut along the imaginary axis leads to

$$F_{\rm i}(T > T_{\rm K}) = -T \ln \left[\frac{\sinh(H/2T)(2s+1)}{\sinh H/2T} \right] + T \int_0^\infty {\rm d}t \frac{B_{2s}(2\pi t, T/H)}{\cos \pi t} t^{-t} \exp(-2t \ln T/T_{\rm K}). \tag{21.169}$$

Here, the poles of $1/\cos(\pi t)$ are compensated by the zeros of $B_{2s}(2\pi t)$. The invariant charge $z(T/T_{\rm K}) > 0$ is now defined by the Gell-Mann-Low equation

$$\frac{1}{z} - \frac{1}{2} \ln z = \ln \left(\frac{T}{T_{\rm K}} \right), \quad z = \frac{1}{\ln(T/T_{\rm K})} + \frac{1}{2 \ln^2 (T/T_{\rm K})} \ln \left[\ln(T/T_{\rm K}) \right] + \cdots . \tag{21.170}$$

The integral term in (21.169) can be expressed by using z as follows

$$Tz \int_0^\infty {\rm d}t \frac{B_{2s}(2\pi z t, T/H)}{\cos \pi z t} \exp(-2t - zt \ln t) = \sum_{n=1}^\infty \beta_n(T/H, s) z^n. \tag{21.171}$$

If $T < T_{\rm K}$, the integration contour in (21.157) is closed in the upper half-plane. The main contribution comes from the cut along the imaginary axis, while the contributions from the poles of $1/\cosh(\omega/2)$ are exponentially small. Introducing the invariant charge $z(T/T_{\rm K}) < 0$ via the equation

$$\frac{1}{z} - \frac{1}{2} \ln |z| = \ln \left(\frac{T}{T_{\rm K}} \right), \tag{21.172}$$

we have

$$F_{\rm i}(T < T_{\rm K}) = -T \ln \left[\frac{\sinh(sH/T)}{\sinh H/2T} \right] + \sum_{n=1}^\infty \beta_n(T/H, s - 1/2) z^n. \tag{21.173}$$

It is seen that, in analogy with the ground state, the high- and low-temperature logarithmic expansions are dual [28].

The above analysis is general. In what follows, we shall derive the leading orders of the high-temperature and low-temperature expansions in detail.

21.7.1 High-temperature expansion

For high temperatures, the zeroth orders of $C_n(\Lambda)$ are their $\Lambda \to \pm\infty$ asymptotics (21.165), i.e.

$$C_n^{(0)}(\Lambda) = \begin{cases} 2 \ln \Phi_n & \text{for } \Lambda < 0, \\ 2 \ln \Phi_{n-1} & \text{for } \Lambda > 0 \text{ and } n > 1. \end{cases} \tag{21.174}$$

Since $\Phi_n^2 = 1 + \Phi_{n-1}\Phi_{n+1}$, these C_n's satisfy the chain of equations (21.156). The way in which the function $C_1(\Lambda)$ vanishes as $\Lambda \to \infty$ follows from the $n = 1$ version of Eq. (21.156):

$$C_1^{(0)}(\Lambda) = \ln \left[1 + \Phi_1 \exp\left(-{\rm e}^{\pi\Lambda} \right) \right] \qquad \text{for } \Lambda > 0. \tag{21.175}$$

In the next order, we set

$$C_n(\Lambda) = C_n^{(0)}(\Lambda) + d_n(\Lambda) \tag{21.176}$$

with a small perturbation $d_n(\Lambda)$. We linearize Eqs. (21.156) in d_n and go to the $\pm$ Fourier space

$$\hat{d}_n^+(\omega) = \int_0^\infty \mathrm{d}\Lambda\, \exp(-\mathrm{i}\omega\Lambda) d_n(\Lambda), \quad \hat{d}_n^-(\omega) = \int_{-\infty}^0 \mathrm{d}\Lambda\, \exp(-\mathrm{i}\omega\Lambda) d_n(\Lambda). \tag{21.177}$$

Thus we obtain

$$\begin{aligned}
\frac{\Phi_n^2}{\Phi_{n-1}\Phi_{n+1}} d_n^- + \frac{\Phi_{n-1}^2}{\Phi_{n-2}\Phi_n} d_n^+ &= s * (d_{n-1} + d_{n+1}), \qquad n \geq 3, && (21.178)\\
\frac{\Phi_2^2}{\Phi_1\Phi_3} d_2^- + \frac{\Phi_1^2}{\Phi_2} d_2^+ &= s * (d_3 + d_1^-) + Y_-, && (21.179)\\
\frac{\Phi_1^2}{\Phi_2} d_1^- &= s * d_2^- + Y_+, && (21.180)
\end{aligned}$$

where

$$\begin{aligned}
\hat{Y}_-(\omega) &= \int_0^\infty \mathrm{d}\Lambda\, \mathrm{e}^{-\mathrm{i}\omega\Lambda} \left[\mathrm{e}^{s*C_1^{(0)}(\Lambda)} - 1\right] \simeq \frac{\mathrm{i}}{\omega - \mathrm{i}0},\\
\hat{Y}_+(\omega) &= \int_{-\infty}^0 \mathrm{d}\Lambda\, \mathrm{e}^{-\mathrm{i}\omega\Lambda} \left(\mathrm{e}^{-\mathrm{e}^{\pi\Lambda}} - 1\right) \simeq \frac{-\mathrm{i}}{\omega + \mathrm{i}0} && (21.181)
\end{aligned}$$

near $\omega = 0$. By construction, the function of interest $\hat{D}_n(\omega)$ in (21.166) is related to $d_n = d_n^+ + d_n^-$ via

$$\hat{D}_n(\omega) = \hat{d}_n(\omega) + O(\omega^3). \tag{21.182}$$

Let us neglect the mutual influence of the regions $\Lambda < 0$ and $\Lambda > 0$ and leave in Eqs. (21.178)-(21.180) only terms with either d_n^+ or d_n^-. In this way we get

$$\begin{aligned}
\frac{\Phi_n^2}{\Phi_{n-1}\Phi_{n+1}} d_n^- &= s * (d_{n-1}^- + d_{n+1}^-),\\
\frac{\Phi_1^2}{\Phi_2} d_1^- &= s * d_2^- + Y_+, && (21.183)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\Phi_{n-1}^2}{\Phi_{n-2}\Phi_n} d_n^+ &= s * (d_{n-1}^+ + d_{n+1}^+),\\
\frac{\Phi_1^2}{\Phi_2} d_2^+ &= s * d_3^+ + Y_-. && (21.184)
\end{aligned}$$

We see that $\hat{d}_{n+1}(\omega) = \hat{d}_n(-\omega)$ in the actual perturbation order, so the duality (21.167) takes place.

The recurrence equations (21.183) and (21.184) are identical to those obtained in the high-temperature treatment of the XXX Heisenberg chain in Sect. 16.2. Their solution is

$$\hat{d}_n^-(\omega) = \frac{2\cosh(\omega/2)}{\Phi_1\Phi_n}\frac{\mathrm{i}}{\omega - \mathrm{i}0}\left[\Phi_{n+1}\mathrm{e}^{-n|\omega|/2} - \Phi_{n-1}\mathrm{e}^{-(n+2)|\omega|/2}\right]. \tag{21.185}$$

The discontinuity of $\hat{d}_n(\omega)$, and therefore $\hat{D}_n(\omega)$, when passing through the point $\omega = 0$ can be evaluated with the aid of Eqs. (21.92) and (21.93). For $n = 2s$, in the limit $H/T \to 0$ the final result is

$$\mathrm{Disc}\,\hat{D}_{2s}(-\mathrm{i}|\omega|, H/T \to 0) = \frac{2}{3}s(s+1)\left[\left(\frac{H}{T}\right)^2 - \omega^2\right]\left(1 - \frac{\omega}{2\pi}\ln|\omega|\right). \tag{21.186}$$

This formula determines the function of interest $\hat{B}_{2s}(\omega, T/H)$ via (21.168). The impurity part of the free energy reads

$$F_{\mathrm{i}}(T) = \begin{cases} -T\ln(2s+1) - T\frac{s(s+1)}{3}f(T/T_{\mathrm{K}}) & \text{for } T \gg T_{\mathrm{K}}, \\ -T\ln 2s - T\frac{s^2-1/4}{3}f(T/T_{\mathrm{K}}) & \text{for } T \ll T_{\mathrm{K}}, \end{cases} \tag{21.187}$$

where

$$f(x) = \frac{H^2}{2T^2}\left(1 - \frac{1}{\ln x}\right) - \frac{\pi^2}{\ln^3 x}. \tag{21.188}$$

21.7.2 Low-temperature expansion

The analysis of the chain of TBA equations (21.126) for the Kondo model resembles that of TBA equations for the antiferromagnetic XXX Heisenberg chain in Sect. 16.3.2. From the structure of TBA equations we deduce that all $\epsilon_n(\Lambda)$ with $n \geq 2$ are positive. Introducing $\epsilon_1^+ = (\epsilon_1 + |\epsilon_1|)/2$, in the small-$T$ limit we have

$$T\ln\left(1 + \mathrm{e}^{\epsilon_1/T}\right) \sim \epsilon_1^+, \qquad T\ln\left(1 + \mathrm{e}^{\epsilon_n/T}\right) \sim \epsilon_n \quad \text{for } n \geq 2. \tag{21.189}$$

• $T = 0$**:** We first consider the leading $T \to 0$ order, $\epsilon_n = \epsilon_n^{(0)}$. $\epsilon_1^{(0)}(\Lambda)$ is positive for $\Lambda < -Q$, vanishes at $\Lambda = -Q$ and is negative for $\Lambda > -Q$. Using the small-T expressions (21.189), the TBA equations (21.126) take the form

$$\begin{aligned} \epsilon_1^{(0)}(\Lambda) &= -\frac{2\varepsilon_{\mathrm{F}}}{\pi}\arctan\left(\mathrm{e}^{\pi\Lambda}\right) + s * \epsilon_2^{(0)}(\Lambda), \\ \epsilon_2^{(0)}(\Lambda) &= s * \epsilon_1^{(0)+}(\Lambda) + s * \epsilon_3^{(0)}(\Lambda), \\ \epsilon_n^{(0)}(\Lambda) &= s * \epsilon_{n-1}^{(0)}(\Lambda) + s * \epsilon_{n+1}^{(0)}(\Lambda), \qquad n \geq 3. \end{aligned} \tag{21.190}$$

The explicit solution of this infinite chain reads

$$\epsilon_n^{(0)}(\Lambda) = H(n-1) + a_{n-1} * \epsilon_1^{(0)+}(\Lambda) \qquad n \geq 2 \tag{21.191}$$

$$\epsilon_1^{(0)}(\Lambda) = -\frac{2\varepsilon_{\mathrm{F}}}{\pi}\arctan\left(\mathrm{e}^{\pi\Lambda}\right) + \frac{H}{2} + (s * a_1) * \epsilon_1^{(0)+}(\Lambda). \tag{21.192}$$

Taking into account that $\hat{s}(\omega)\hat{a}_1(\omega) = -\hat{J}(\omega)$, with J defined in Eq. (21.80), $\epsilon_1^{(0)}(\Lambda)$ satisfies the integral equation

$$\epsilon_1^{(0)}(\Lambda) + \int_{-\infty}^{-Q} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda')\epsilon_1^{(0)}(\Lambda') = -\frac{2\varepsilon_{\mathrm{F}}}{\pi}\arctan\left(\mathrm{e}^{\pi\Lambda}\right) + \frac{H}{2}. \tag{21.193}$$

We want to have as a reference the Fermi point $-Q$, defined by (21.97). In the scaling limit $\varepsilon_{\mathrm{F}} \to \infty$, the integral equation (21.193) becomes

$$\epsilon_1^{(0)}(\Lambda-Q) + \int_{-\infty}^{0} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda')\epsilon_1^{(0)}(\Lambda'-Q) = -H\sqrt{\frac{\mathrm{e}}{2\pi}}\mathrm{e}^{\pi\Lambda} + \frac{H}{2}, \qquad \Lambda < 0. \tag{21.194}$$

To solve this equation we apply the Wiener-Hopf analysis which follows Eq. (21.87). Now the Fourier transform of the rhs function

$$g(\Lambda) = \begin{cases} -H\sqrt{\frac{\mathrm{e}}{2\pi}}\mathrm{e}^{\pi\Lambda} + \frac{H}{2}, & \text{for } \Lambda < 0, \\ 0 & \text{for } \Lambda > 0 \end{cases} \tag{21.195}$$

is

$$\hat{g}(\omega) = -H\sqrt{\frac{\mathrm{e}}{2\pi}}\frac{1}{\mathrm{i}\omega+\pi} + \frac{H}{2}\frac{1}{\mathrm{i}\omega+0}.$$

The poles of $\hat{g}(\omega)$ at $\omega = \mathrm{i}0$ and $\omega = \mathrm{i}\pi$ are removed by subtracting residues in the combination

$$F_+(\omega)\hat{g}(\omega) \to -H\sqrt{\frac{\mathrm{e}}{2\pi}}\frac{F_+(\mathrm{i}\pi)}{\mathrm{i}\omega+\pi} + \frac{H}{2}\frac{F_+(0)}{\mathrm{i}\omega+0} = -H\frac{\pi}{\sqrt{2}}\frac{1}{(\omega-\mathrm{i}0)(\omega-\mathrm{i}\pi)}. \tag{21.196}$$

Thus, using (21.191), we obtain

$$\epsilon_n^{(0)}(\Lambda-Q) = -\frac{H}{2^{3/2}}\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{F_-(\omega)}{(\omega-\mathrm{i}0)(\omega-\mathrm{i}\pi)}\mathrm{e}^{-\mathrm{i}\omega\Lambda-(n-1)|\omega|/2} + (n-1)H \tag{21.197}$$

for all $n = 1, 2, \ldots$.

• **Small T:** In the next order of TBA equations (21.126), the contribution of the exponentials $\exp(-\epsilon_n^{(0)}/T)$ with $n \geq 2$ is negligible. We have to substitute $\epsilon_1^{(0)+} \to T\ln(1+\mathrm{e}^{\epsilon_1/T})$ in Eqs. (21.191) and (21.192), to obtain

$$\epsilon_n(\Lambda) = H(n-1) + a_{n-1} * T\ln\left[1+\mathrm{e}^{\epsilon_1(\Lambda)/T}\right], \qquad n \geq 2 \tag{21.198}$$

and

$$\epsilon_1(\Lambda) + T\int_{-\infty}^{\infty}\mathrm{d}\Lambda'\, J(\Lambda-\Lambda')\ln\left[1+\mathrm{e}^{\epsilon_1(\Lambda')/T}\right] = -\frac{2\varepsilon_{\mathrm{F}}}{\pi}\arctan\left(\mathrm{e}^{\pi\Lambda}\right) + \frac{H}{2}. \tag{21.199}$$

We use the trick formula

$$T\ln\left[1+\mathrm{e}^{\epsilon_1(\Lambda)/T}\right] = T\ln\left[1+\mathrm{e}^{-|\epsilon_1(\Lambda)|/T}\right] + \epsilon_1^+(\Lambda). \tag{21.200}$$

The zero point of ϵ_1, temperature-dependent Q_T, can be substituted in the considered T-order by its $T=0$ value Q. Writing $\epsilon_1 = \epsilon_1^{(0)} + \epsilon_1^{(1)}$ in (21.199) and subtracting the linearized Eq. (21.193), the first correction $\epsilon_1^{(1)}$ satisfies the integral equation

$$\epsilon_1^{(1)}(\Lambda) + \int_{-\infty}^{-Q} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda')\epsilon_1^{(1)}(\Lambda') = I(\Lambda), \tag{21.201}$$

where the inhomogeneous term $I(\Lambda)$ is given by

$$I(\Lambda) = -T\int_{-\infty}^{\infty} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda') \ln\left[1+\mathrm{e}^{-|\epsilon_1(\Lambda')|/T}\right]. \tag{21.202}$$

The dominant contribution to $I(\Lambda)$ comes from the neighborhood of zero of ϵ_1. Expanding $\epsilon_1(\Lambda)$ around $\Lambda=-Q$, $\epsilon_1(\Lambda) \sim \epsilon_1^{(0)'}(-Q)(\Lambda+Q)$, the leading T-dependence of $I(\Lambda)$ reads

$$I(\Lambda) = -\frac{\pi^2 T^2}{6|\epsilon_1^{(0)'}(-Q)|} J(\Lambda+Q). \tag{21.203}$$

Hence

$$\epsilon_1^{(1)}(\Lambda) = \frac{\pi^2 T^2}{6|\epsilon_1^{(0)'}(-Q)|} C(\Lambda), \tag{21.204}$$

where $C(\Lambda)$ satisfies the integral equation

$$C(\Lambda) + \int_{-\infty}^{-Q} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda')C(\Lambda') = -J(\Lambda+Q). \tag{21.205}$$

The free energy of the impurity (21.149) is expressed as

$$F_{\mathrm{i}}(T,H) = -\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, s(\Lambda+1/g)\epsilon_{2s}(\Lambda), \tag{21.206}$$

where $\epsilon_{2s}(\Lambda)$ is given by (21.198). Using the formula (21.200) and the relation $\hat{a}_{2s-1}(\omega)\hat{s}(\omega) = \hat{\mathcal{S}}_{2s}(\omega)$ [see definition (21.80)], we find

$$\begin{aligned} F_{\mathrm{i}}(T,H) - F_{\mathrm{i}}(0,H) &= -T\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \mathcal{S}_{2s}(\Lambda+1/g) \ln\left[1+\mathrm{e}^{-|\epsilon_1^{(0)}(\Lambda)|/T}\right] \\ &\quad + \int_{-\infty}^{-Q} \mathrm{d}\Lambda\, \mathcal{S}_{2s}(\Lambda+1/g)\epsilon_1^{(1)}(\Lambda). \end{aligned} \tag{21.207}$$

The rhs of this equation is expressible as

$$-\frac{\pi^2 T^2}{6|\epsilon_1^{(0)'}(-Q)|}\left[\mathcal{S}_{2s}(-Q+1/g) + \int_{-\infty}^{-Q} \mathrm{d}\Lambda\, \mathcal{S}_{2s}(\Lambda+1/g)C(\Lambda)\right].$$

Introducing the function $V(\Lambda)$ as the solution of the integral equation

$$V(\Lambda) + \int_{-\infty}^{-Q} \mathrm{d}\Lambda'\, J(\Lambda-\Lambda')V(\Lambda') = \mathcal{S}_{2s}(\Lambda+1/g), \tag{21.208}$$

the expression in the square bracket is nothing but $V(-Q)$. We conclude that in the leading T-order

$$F_{\rm i}(T,H)-F_{\rm i}(0,H)=-\frac{\pi^2T^2}{6|\epsilon_1^{(0)'}(-Q)|}V(-Q). \tag{21.209}$$

Comparing the integral equation (21.208) with (21.79) we see that $V(\Lambda)=\tilde{r}_{\rm i}(\Lambda+Q)$, i.e. $V(-Q)=\tilde{r}_{\rm i}(0)$. Using the analogy of (14.34) (the contour in now closed in Π_-), Eqs. (21.102) and (21.103) imply

$$\tilde{r}_{\rm i}(0)=\lim_{|\omega|\to\infty}{\rm i}\omega\hat{\tilde{r}}_{\rm i}(\omega)=\int_{-\infty}^{\infty}\frac{{\rm d}\omega'}{2\pi}\varphi(\omega')F_+(\omega'+{\rm i}0)=\sqrt{2}H\pi\chi_{\rm i}(H/T_H), \tag{21.210}$$

where $\chi_{\rm i}=\partial M_{\rm i}/\partial H$ is the susceptibility. To obtain $\epsilon_1^{(0)'}(-Q)$, we differentiate Eq. (21.194) with respect to Λ and then perform integration by parts in the integral over Λ' [$\epsilon_1^{(0)}(-Q)=0$], with the result

$$\epsilon_1^{(0)'}(\Lambda-Q)+\int_{-\infty}^{0}{\rm d}\Lambda'\,J(\Lambda-\Lambda')\epsilon_1^{(0)'}(\Lambda'-Q)=-H\sqrt{\frac{\pi{\rm e}}{2}}{\rm e}^{\pi\Lambda}. \tag{21.211}$$

Comparing this integral equation with (21.87) we find that $\epsilon_1^{(0)'}(\Lambda-Q)=-H\sqrt{\pi{\rm e}/2}\tilde{r}^{(0)}(\Lambda)$, i.e. $\epsilon_1^{(0)'}(-Q)=-H\sqrt{\pi{\rm e}/2}\tilde{r}^{(0)}(0)$. From (21.96) we get

$$\tilde{r}^{(0)}(0)=\lim_{|\omega|\to\infty}{\rm i}\omega\hat{\tilde{r}}^{(0)}(\omega)=F_+({\rm i}\pi)=\sqrt{\frac{\pi}{\rm e}}. \tag{21.212}$$

Consequently,

$$F_{\rm i}(T,H)-F_{\rm i}(0,H)=-\frac{\pi^2T^2}{3}\chi_{\rm i}(H/T_H) \tag{21.213}$$

and we arrive at the Wilson-Nozières formula for Fermi liquids

$$\frac{1}{T}C_{\rm i}(H/T_{\rm K})=\frac{2\pi^2}{3}\chi_{\rm i}(H/T_{\rm K}) \tag{21.214}$$

valid for an arbitrary magnetic field.

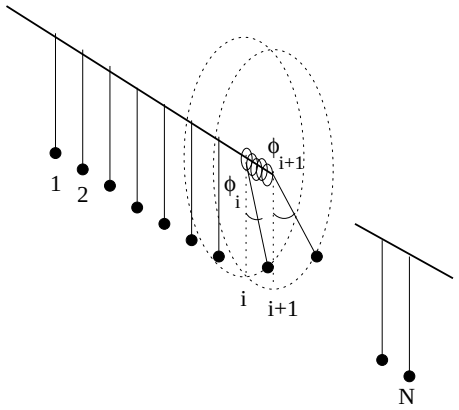
QUANTUM FIELD THEORY: SINE-GORDON MODEL

22 Classical sine-Gordon theory

In this section, the classical sine-Gordon theory is reviewed. It is introduced as a continuum (infinite dimensional) limit of a finite dimensional mechanical system. Then some related continuum field theories are discussed: the Klein-Gordon theory as the non-interacting limit, the sinh-Gordon theory as its analytical continuation and the corresponding Euclidean counterparts. Then we turn to the construction of the finite energy solutions of the sine-Gordon theory [35]. We start with the static solutions: The soliton and the anti-soliton. By boosting them up we can interpret these solutions as moving particles. States with more particles can be generated by the Bäcklund transformation. We construct two-particle solutions and introduce the concept of time shifts. Finally, general finite energy solutions are reviewed and the integrability of the model is shown.

22.1 Continuum limit of a mechanical system

Consider a mechanical system composed of N coupled pendula in a vertical gravitational field of strength g:



Let us denote the angular coordinate of the ith pendulum by ϕ_i, its length by l and mass by μ. Neighbouring pendula, placed at distance a, are coupled via a harmonic potential of tension k. The Lagrangian of this finite-dimensional system is given by[3]

$$L = E_{\rm kin} - E_{\rm pot} = \sum_{i=1}^{N} \left[\frac{1}{2}\mu l^2 \dot{\phi}_i^2 - \frac{1}{2}k(\phi_i - \phi_{i+1})^2 \right] - \sum_{i=1}^{N} \mu g l (1 - \cos\phi_i). \qquad (22.1)$$

We are interested in the continuum limit $a \to 0$ and $N \to \infty$, keeping the length of the system $L = Na$ fixed. For this purpose we introduce the continuum variable

$$\varphi\left((i-1)a\right) = \frac{\phi_i}{b}; \qquad \frac{m^2}{b^2} = \frac{\mu g l}{a} \qquad (22.2)$$

[3] We have to specify also the boundary conditions: we can take periodic, free, or the fixed one.

and, in the continuum limit, set the scale $\mu l^2\beta^2/a = k\beta^2 a = 1$. As the result, we obtain the Lagrangian of the sine-Gordon theory

$$L = \int_0^L \mathrm{d}x\, \mathcal{L} = \int_0^L \mathrm{d}x\, \left[\frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - \frac{m^2}{b^2}(1-\cos b\varphi)\right], \tag{22.3}$$

where $\partial_t\varphi \equiv \partial\varphi/\partial t$, $\partial_x\varphi \equiv \partial\varphi/\partial x = \lim_{a\to 0}[\varphi(x+a)-\varphi(x)]/a$ and the speed of light is normalized to 1. The minimality of the action

$$\delta S = 0; \qquad S[\varphi] = \int \mathrm{d}t \int \mathrm{d}x\, \mathcal{L}(\varphi, \partial_t\varphi, \partial_x\varphi) \tag{22.4}$$

determines the equation of motion

$$\partial_t \frac{\partial\mathcal{L}}{\partial(\partial_t\varphi)} + \partial_x \frac{\partial\mathcal{L}}{\partial(\partial_x\varphi)} - \frac{\partial\mathcal{L}}{\partial\varphi} = (\partial_t^2 - \partial_x^2)\varphi + V'(\varphi) = 0. \tag{22.5}$$

If we normalize the action to be dimensionless ($\hbar = 1$), then the scalar field φ and the parameter b are also dimensionless and m determines the energy scale.

Let us emphasize that, firstly, the finite-dimensional system has more parameters than the continuum one and, secondly, the field theory is obtained as a singular limit $k \to \infty$, $N \to \infty$ of a well-defined finite system. This singular limit would lead to singularities when we would like to quantize the system.

22.2 Related models

Here we list some models which are related to the sine-Gordon theory.

22.2.1 Sinh-Gordon theory

If we analytically continue the parameter $b \to \mathrm{i}b$, we obtain the Lagrangian of the sinh-Gordon theory

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - \frac{m^2}{b^2}(\cosh b\varphi - 1). \tag{22.6}$$

In contrast to the sine-Gordon theory, where the field φ lives on a compact space (the circle), the sinh-Gordon field lives on the non-compact full line. The space where the fields take values is usually called the target space. Thus the target space of the sine-Gordon theory is $\mathbb{S}^1$ while the target space of the sinh-Gordon theory is $\mathbb{R}$. These topologically different spaces will lead to drastic differences between the models, both at the classical and quantum levels.

22.2.2 Klein-Gordon equation

The parameter b in the sinh- or sine-Gordon theory can be interpreted as a coupling constant. Indeed, taking the $b \to 0$ limit in (22.6) we obtain a weakly coupled theory

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - \frac{m^2}{2}\varphi^2 - \frac{m^2b^2}{4!}\varphi^4 - \cdots. \tag{22.7}$$

For $b = 0$ the theory is actually free and we obtain the Klein-Gordon model. The method of the least action gives the relativistic wave equation

$$(\partial_t^2 - \partial_x^2 + m^2)\varphi \equiv \Box_x \varphi = 0 \tag{22.8}$$

as the equation of motion. It was discovered by Schrödinger in order to describe the spectrum of the Hydrogen atom (and rejected by himself as it wrongly reproduced the fine-structure[4]). The Klein-Gordon model is relativistically invariant which means that the equation of motion is covariant under Lorentz transformation:

$$\Box_x = \Box_{x'}; \qquad x' = (x - vt)\gamma, \qquad t' = (t - vx)\gamma, \qquad \gamma^{-1} = \sqrt{1 - v^2} \tag{22.9}$$

($|v| < 1$) and is invariant under space $x' = x + x_0$ and time $t' = t + t_0$ translations. The Lorentz transformation takes a particularly simple form in the rapidity parameterization

$$v = \tanh \Lambda; \qquad x' = x \cosh \Lambda - t \sinh \Lambda, \qquad t' = t \cosh \Lambda - x \sinh \Lambda, \tag{22.10}$$

which is nothing but a hyperbolic rotation. Light-cone coordinates diagonalize this transformation,

$$x_\pm = \frac{1}{2}(t \pm x); \qquad x'_\pm = \mathrm{e}^{\pm\Lambda} x_\pm. \tag{22.11}$$

22.2.3 Euclidean version

The Euclidean version of a relativistic field theory defined by the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial_t \varphi)^2 - \frac{1}{2}(\partial_x \varphi)^2 - V(\varphi) \tag{22.12}$$

means an analytical continuation in the time coordinate $t \to y = \mathrm{i}t$. The resulting Euclidean action S_E is positive definite, if the potential V is bounded from below:

$$S = \int \mathrm{d}t \int \mathrm{d}x\, \mathcal{L} \to -S_E = -\int \mathrm{d}y \int \mathrm{d}x \left\{ \frac{1}{2}\left[(\partial_x \varphi)^2 + (\partial_y \varphi)^2\right] + V(\varphi) \right\}. \tag{22.13}$$

The Lorentz invariance translates in the continued theory to the rotational invariance in the Euclidean (x, y) plane.

22.3 Finite energy solutions

The sine-Gordon model with the potential

$$V(\varphi) = \frac{m^2}{\beta^2}(1 - \cos \beta\varphi) \tag{22.14}$$

is also relativistically invariant. From its invariance under time translations the conservation of energy follows[5]

$$E[\varphi] = \int_0^L \mathrm{d}x \left[\frac{1}{2}(\partial_t \varphi)^2 + \frac{1}{2}(\partial_x \varphi)^2 + V(\varphi) \right]. \tag{22.15}$$

[4] For more details see http://en.wikipedia.org/wiki/Klein-Gordon_equation.

[5] Periodic BC is understood.

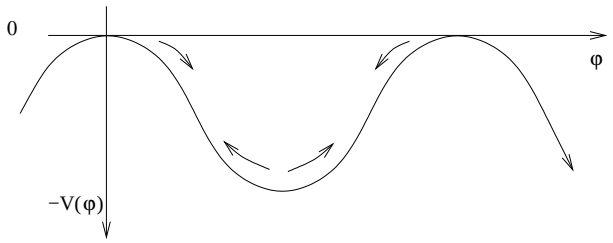


Fig. 22.1. Static solutions can be interpreted as the motion of a particle in the $U = -V$ potential. Finite energy configurations in the infinite volume limit interpolate between neighbouring minima of V.

This conserved energy of the field theory is a functional of the field configurations. The invariance under space translations leads to the conserved momentum functional:

$$P[\varphi] = \int_0^L \mathrm{d}x \; [\partial_x \varphi \partial_t \varphi] \,. \tag{22.16}$$

We are interested in configurations which have finite energy and momentum.

22.3.1 One-particle solutions

Symmetries are useful in two respects: first, they give rise to conserved charges (which generate the symmetries themselves), second, they map solutions of the equation of motion to other solutions. By exploiting the relativistic invariance we can generate time-dependent solutions from the static ones.

The static equation reads as

$$(\partial_t^2 - \partial_x^2)\varphi + V'(\varphi) = 0 \quad \longrightarrow \quad -\partial_x^2 \varphi + V'(\varphi) = 0. \tag{22.17}$$

It is analogous to the Newton's equation of motion for a particle in one-dimensional potential $U(r) = -(m^2/b^2)(1 - \cos br)$:

$$\frac{\mathrm{d}^2 r}{\mathrm{d}\tau^2} = -U'(r) \quad \longleftrightarrow \quad \frac{\mathrm{d}^2 \varphi}{\mathrm{d}x^2} = V'(\varphi). \tag{22.18}$$

The coordinate of the one-dimensional motion is denoted by r while its time variable by τ. The correspondence reads as $r \leftrightarrow \varphi$, $\tau \leftrightarrow x$, $U \leftrightarrow -V$. We can exploit the conservation of the energy of the point particle $\epsilon = (1/2)(\mathrm{d}r/\mathrm{d}\tau)^2 + U(r)$ to integrate the static equation of motion

$$\tau = \int \frac{\mathrm{d}r}{\pm\sqrt{2[\epsilon - U(r)]}} + \tau_0 \quad \longleftrightarrow \quad x = \int \frac{\mathrm{d}\varphi}{\pm\sqrt{2[\epsilon + V(\varphi)]}} + x_0. \tag{22.19}$$

For the sine-Gordon potential (22.14), we obtain the representation by elliptic integrals.

The infinite volume limit, however, simplifies considerably:

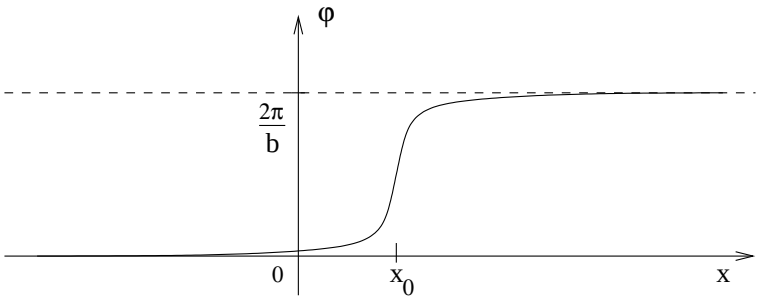


Fig. 22.2. The static soliton solution φ_s interpolates between 0 and $2\pi/b$.

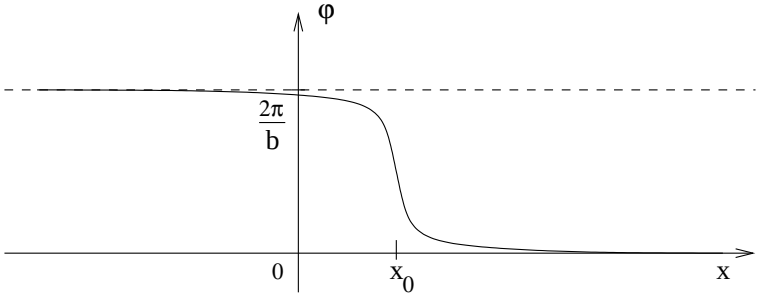


Fig. 22.3. The static anti-soliton solution $\varphi_{\bar{s}}$ interpolates between $2\pi/b$ and 0.

The finiteness of the energy of the field configuration, $E[\varphi] < \infty$, requires that $\partial_x\varphi \to 0$, $V(\varphi) \to 0$ as $x \to \pm\infty$. Taking a look at the movement of the analogue particle in the U potential, Fig. 22.1, we can see that at negative and positive infinite times the particle has to be on the top of the potential. That is the point where particle's energy has to vanish, $\epsilon = 0$, giving rise to

$$x - x_0 = \pm \int \frac{\mathrm{d}\varphi}{\sqrt{2V(\varphi)}} = \pm \int \frac{\mathrm{d}(b\varphi/2)}{m \sin(b\varphi/2)} = \pm \frac{1}{m} \ln\left(\tan\left(\frac{b\varphi}{4}\right)\right). \tag{22.20}$$

The two $\pm$ solutions

$$\varphi_s(x) = \frac{4}{b} \arctan\left(\mathrm{e}^{m(x-x_0)}\right), \qquad \varphi_{\bar{s}}(x) = \frac{4}{b} \arctan\left(\mathrm{e}^{-m(x-x_0)}\right) \tag{22.21}$$

are called the soliton and the anti-soliton, respectively. The soliton interpolates between 0 and $2\pi/b$ as x moves from $-\infty$ to ∞, the anti-soliton interpolates oppositely. They are shown in Figs. 22.2 and 22.3. Clearly the sinh-Gordon potential has only one minimum, so this theory does not allow for nontrivial static solutions.

We can use the energy functional of the sine-Gordon theory (22.15) to calculate the energy of the solutions. Both solutions have the energy

$$E[\varphi_s] = E[\varphi_{\bar{s}}] = \frac{8m}{b^2} \equiv M_0 \tag{22.22}$$

which, from now on, we denote by M_0. For static solutions the momentum (22.16) vanishes, $P = 0$. Notice that the two static solutions are nonperturbative in the sense that they become infinitely heavy in the weakly coupled limit $b \to 0$.

Since the equation of motion is relativistically invariant, static solutions can be viewed by a moving observer. For the moving observer these static solutions acquire a very specific time-dependence:

$$\varphi(x,t) = \varphi_s\left((x-vt)\gamma\right) = \frac{4}{b}\arctan\left(\mathrm{e}^{m\gamma(x-vt-x_0)}\right), \tag{22.23}$$

where we redefined x_0 and, as before, $\gamma^{-1} = \sqrt{1-v^2}$. This provides a time dependent solution of the equation of motion. The conserved energy (22.15) and momentum (22.16) of the moving soliton configuration (22.23) read

$$E[\varphi_s((x-vt)\gamma)] \equiv E(v) = \frac{M_0}{\sqrt{1-v^2}}, \quad P[\varphi_s((x-vt)\gamma)] \equiv P(v) = \frac{M_0 v}{\sqrt{1-v^2}}. \tag{22.24}$$

Clearly, these quantities are related to one another like the relativistic energy and momentum of a moving particle whose velocity is v. For any relativistic particle the mass-shell condition is satisfied

$$E(v)^2 - P(v)^2 = M_0^2, \tag{22.25}$$

where M_0 is the mass of the particle. As a consequence, momentum and energy are not independent and we can parameterize a moving relativistic particle by its rapidity θ as

$$E(\theta) = M_0\cosh\theta, \qquad P(\theta) = M_0\sinh\theta, \qquad v = \tanh\theta. \tag{22.26}$$

The rapidity is a convenient parameter as the Lorentz transformation (22.10) merely shifts its value $\theta' = \theta + \Lambda$.

The moving soliton and anti-soliton solutions behave like solitary waves, i.e. waves that travel alone keeping their shapes forever. That is why they are called soliton and anti-soliton. The soliton and the anti-soliton have localized energy density and, due to the non-linearity of the sine-Gordon equation, they are dispersionless solutions.

The energy densities of the soliton and of the anti-soliton are the same, the only difference consists in their topological charge:

$$Q_{\mathrm{top}} = \frac{2\pi}{b}\int_{-\infty}^{\infty}\partial_x\varphi(x,t)\mathrm{d}x = \frac{2\pi}{b}\left[\varphi(\infty) - \varphi(-\infty)\right]. \tag{22.27}$$

As time evolution is a continuous deformation of the field configurations, the topological charge is a conserved quantity in any one-dimensional field theory. Within our normalization, it takes ± 1 for the soliton/anti-soliton solutions, respectively. Solitons and anti-solitons are localized objects which we treat as particles. This is also suggested by their dispersion relation. Now we analyze the interaction of these particles.

22.4 Scattering solutions, time shifts

In order to analyze the interaction of the soliton and anti-soliton "particles", we need some exact solutions which contain more than just one particle. Because the sine-Gordon equation (22.5) is nonlinear, we cannot just simply add two solitons. But the very remarkable so-called Bäcklund transformation will exactly do this job [36].

22.4.1 Bäcklund transformation

The Bäcklund transformation in its most "naive" form tells us how to reconstruct the imaginary part v of a holomorphic function f from its real part u. Indeed, if u is harmonic, i.e. $(\partial_x^2+\partial_y^2)u = 0$, and u and v satisfy the Cauchy-Riemann equations $\partial_x u = \partial_y v$ and $\partial_y u = -\partial_x v$, then v is harmonic too, $(\partial_x^2 + \partial_y^2)v = 0$. This situation appears for the Euclidean version of the sine-Gordon theory when $m = 0$. The specialty about the sine-Gordon theory is that this construction can be extended to non-vanishing m. The extension of this Bäcklund transformation allows us to generate a new solution φ_2 of the sine-Gordon equation (22.5) provided that an initial solution φ_1 is already known. We claim that if φ_1 solves the sine-Gordon equation of motion

$$-\partial_+\partial_-\varphi_1 = \frac{m^2}{b}\sin b\varphi_1, \qquad \partial_\pm = \partial_t \pm \partial_x \tag{22.28}$$

and additionally φ_2 satisfies

$$\begin{aligned} \partial_+\varphi_2 &= \partial_+\varphi_1 + \frac{2m\sigma}{b}\sin\left(\frac{b}{2}(\varphi_1+\varphi_2)\right), \\ \partial_-\varphi_2 &= -\partial_-\varphi_1 + \frac{2m}{b\sigma}\sin\left(\frac{b}{2}(\varphi_1-\varphi_2)\right), \end{aligned} \tag{22.29}$$

then φ_2 also solves the sine-Gordon equation, where σ is a free parameter. These equations are of first order only and so they much easier to be solved than the sine-Gordon equation itself. The existence of the Bäcklund transformation, which is highly nontrivial, is related to the magical integrability property of the model.

22.4.2 Two-particle solutions

If we plug into the Bäcklund transformation the one-particle solution (22.21), we obtain two-particle solutions. Especially for two solitons, we get

$$\varphi_{ss}(x,t) = \frac{4}{b}\arctan\left(\frac{v\sinh(mx\gamma)}{\cosh(mvt\gamma)}\right). \tag{22.30}$$

Similarly, the soliton–anti-soliton solution reads

$$\varphi_{s\bar{s}}(x,t) = \frac{4}{b}\arctan\left(\frac{\sinh(mvt\gamma)}{v\cosh(mx\gamma)}\right). \tag{22.31}$$

Let us analyze this soliton–anti-soliton solution. For asymptotically large times, one of the exponential terms in

$$\varphi_{s\bar{s}}(x,t) = \frac{4}{b}\arctan\left(\frac{\mathrm{e}^{mvt\gamma-\ln v} - \mathrm{e}^{-mvt\gamma-\ln v}}{\mathrm{e}^{mx\gamma}+\mathrm{e}^{-mx\gamma}}\right) \tag{22.32}$$

survives and the solution becomes the sum of two well-separated one-particle solutions. Say, for asymptotically large negative times ($t \to -\infty$, remote past) we can keep the $e^{-mvt\gamma-\ln v}$ term alone. Then we can focus on the domains where the argument changes nontrivially. They are

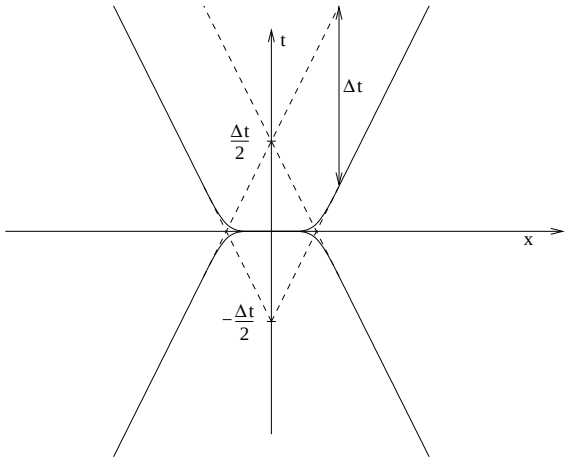


Fig. 22.4. Schematic space-time diagram of the energy density of the soliton–anti-soliton $\varphi_{s\bar{s}}$ solution. In the scattering process the particles acquire speed-dependent time advance $\Delta t = -2\ln v/(mv\gamma)$ showing that their interaction is attractive.

located either for large negative x or for large positive x, where we can keep one exponential in the denominator, too, and obtain:

$$\begin{aligned}\varphi_{s\bar{s}}(x,t) &\approx \varphi_s\left(\left[x+v\left(t-\frac{\Delta t}{2}\right)\right]\gamma\right)+\varphi_{\bar{s}}\left(\left[x-v\left(t-\frac{\Delta t}{2}\right)\right]\gamma\right),\\ &\Delta t=-2\frac{\ln v}{mv\gamma}>0.\end{aligned} \tag{22.33}$$

Thus we have a soliton and an anti-soliton approaching each other with velocity $-v$ and v. For asymptotically large positive times ($t\to\infty$, remote future), we have

$$\varphi_{s\bar{s}}(x,t)\approx\varphi_s\left(\left[x+v\left(t+\frac{\Delta t}{2}\right)\right]\gamma\right)+\varphi_{\bar{s}}\left(\left[x-v\left(t+\frac{\Delta t}{2}\right)\right]\gamma\right). \tag{22.34}$$

The velocities of the particles are not changed and we can interpret $\Delta t>0$ as the time advance experienced by the soliton in the potential of the anti-soliton, see Fig. 22.4.

Since for asymptotic times the two-particle solution is the sum of well-separated one-particle solutions, the energy of the state is simply the sum of the one-particle energies:

$$E[\varphi_{s\bar{s}}(x,t)]=E[\varphi_s((x+vt)\gamma)+E[\varphi_{\bar{s}}(x-vt)\gamma)]=\frac{2M_0}{\sqrt{1-v^2}}=2M_0\cosh\theta. \tag{22.35}$$

The time advance indicates that the soliton–anti-soliton interaction is attractive and therefore we can expect the formation of boundstates. Indeed, continuing analytically the velocity $v\to iu$ in $\varphi_{s\bar{s}}$ we obtain the so-called breather solution

$$\varphi_b(x,t)=\frac{4}{b}\arctan\left(\frac{\sin(mut\gamma)}{u\cosh(mx\gamma)}\right), \tag{22.36}$$

which is periodic in time and possesses one continuous parameter u. The energy (mass) of this standing breather can be obtained from the energy functional

$$E[\varphi_b] = m_b = \frac{2M_0}{\sqrt{1+u^2}} = 2M_0 \cos\vartheta, \tag{22.37}$$

where ϑ is the imaginary rapidity $\theta \to \mathrm{i}\vartheta$ at which the boundstate is formed.

22.4.3 Multiparticle solutions

The generic multiparticle solution can be obtained, in principle, by applying iteratively the Bäcklund transformation and generating from an N particle solution an $N+1$ particle solution. We present the final result in the Hirota form [37]:

$$\varphi = \frac{4}{b} \arctan \frac{\Im m(\tau)}{\Re e(\tau)}, \tag{22.38}$$

where

$$\begin{aligned} \tau \quad = \quad & \sum_{\{\mu_j=0,1\}} \exp\left(-\sum_{j=1}^{N} \mu_j \left[xm\cosh\theta_j + tm\sinh\theta_j - x_j - \frac{\mathrm{i}\pi}{2}\epsilon_j \right] \right. \\ & \left. +2\sum_{i<j} \mu_i\mu_j \ln\left(\frac{\tanh(\theta_i-\theta_j)}{2} \right) \right). \end{aligned} \tag{22.39}$$

For states containing k solitons and $N-k$ anti-solitons we have to put $\epsilon_1 = \ldots = \epsilon_k = 1$ and $\epsilon_{k+1} = \ldots = \epsilon_N = -1$. The sum runs over all possible values of $\{\mu_i | i = 1, \ldots N\}$. The parameter θ_j is the rapidity of the jth particle, while x_j denotes its location. The energy and momentum of such state are given by

$$E[\varphi] = \sum_{j=1}^{N} M_0 \cosh\theta_j, \qquad P[\varphi] = \sum_{j=1}^{N} M_0 \sinh\theta_j. \tag{22.40}$$

States of breather type are constructed as moving soliton–anti-soliton boundstates ($\theta_s = \theta + \mathrm{i}\vartheta, \theta_{\bar{s}} = \theta - \mathrm{i}\vartheta$).

Let us take a look at the structure of the generic solution. In the remote past $t \to -\infty$, the solution is composed of well-separated non-interacting particles of types soliton, anti-soliton and breather, which have different velocities. This initial state can be formally described by

$$A(\theta_1)A(\theta_2)\cdots A(\theta_N), \qquad \theta_1 > \theta_2 > \cdots > \theta_N. \tag{22.41}$$

Here, A denotes the type of the particle: $A = s$ for the soliton, $A = \bar{s}$ for the anti-soliton and $A = B_\vartheta$ for the breather. $\{\theta_i\}$ represents the ordered set of rapidities. In the initial configuration, we ordered one-particle symbols according to their rapidity: The fastest is on the left. In the remote future $t \to \infty$, the particle content is the same even with the same rapidities, except that their ordering is just opposite:

$$A(\theta_N)A(\theta_{N-1})\cdots A(\theta_1), \qquad \theta_1 > \cdots > \theta_{N-1} > \theta_N. \tag{22.42}$$

The only difference compared to the free motion consists in the acquired time shift (advance or delay). The time shift of any particle is the sum of time shifts they would acquire if they had scattered only with one particular constituent. That is if the particle of type i acquires a time shift Δt_{ij} on passing through particle j, which can be extracted from the two-particle solution $\varphi_{ij}(x,t)$ by analyzing its asymptotic, then the total time shift is

$$\Delta t_i = \sum_{j:j\neq i} \Delta t_{ij}. \tag{22.43}$$

This manifestation of the model integrability is called the factorizability of the scattering process.

22.5 Integrability, conserved charges

The dispersionless nature of the solutions and the factorizability of the scatterings are consequences of integrability of the model [29, 30]. Integrability means the existence of an infinite number of commuting conserved charges. In the sequel, we analyze necessary requirements for the existence of conserved "higher-spin" charges.

22.5.1 Conservation laws

Conserved charges originate from conservation laws of the form

$$\partial_\mu K^\mu \equiv \eta^{\mu\nu}\partial_\mu K_\nu = \partial_t K_t - \partial_x K_x = 0, \qquad \eta = \mathrm{diag}(1,-1). \tag{22.44}$$

Indeed, integrating the time component of the conserved current K_t over a space-like surface, the resulting charge

$$Q = \int_{-\infty}^{\infty} K_t(t,x)\mathrm{d}x \tag{22.45}$$

is conserved, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}Q = \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} K_t(t,x)\mathrm{d}x = \int_{-\infty}^{\infty} \partial_t K_t\,\mathrm{d}x = \int_{-\infty}^{\infty} \partial_x K_x\,\mathrm{d}x = 0, \tag{22.46}$$

where we used that the currents vanish at space-like infinities. Clearly, not all conserved currents lead to conserved charges: For a total derivative $K_t = \partial_x \tilde{K}$ the integral vanishes by itself. Sometimes it is better to work in light-cone coordinates. The conservation laws for the current light-cone components read as

$$\partial_+ K_- + \partial_- K_+ = 0, \qquad K_\pm = \frac{1}{2}(K_t \pm K_x). \tag{22.47}$$

22.5.2 Conserved charges in the free theory

Let us come back to the original problem and try to find conserved charges for the sine-Gordon theory. We start with the free theory

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 = \partial_+\varphi\partial_-\varphi \quad \longrightarrow \quad \partial_+\partial_-\varphi = 0. \tag{22.48}$$

From the equation of motion it follows that $K_- = \partial_-\varphi \equiv J_-$ and $K_+ = 0 \equiv J_+$ will be conserved:

$$\partial_+ J_- + \partial_- J_+ = \partial_+ J_- = \partial_+\partial_-\varphi = 0. \tag{22.49}$$

In an analogous way, we can introduce the two-component current $\bar{J} = (\bar{J}_-, \bar{J}_+) = (0, \partial_+\varphi)$ such that the following conservation law holds:

$$\partial_- \bar{J}_+ = 0. \tag{22.50}$$

According to our previous remark, these currents are not appropriate in the sense that they are total derivatives. The conservation law $\partial_+ J_- = 0$ is still useful as it shows that J_- depends on x_- only. Thus any differential polynomial of J_- will be conserved, too,

$$\partial_+ \left[(\partial_-^{n_1} J_-)(\partial_-^{n_2} J_-)\cdots(\partial_-^{n_k} J_-)\right] = 0. \tag{22.51}$$

Clearly, any statements made about J can be directly generalized to $\bar{J}$ by exchanging $+ \leftrightarrow -$, so from now on we shall focus on J only. As concerns currents which correspond to nontrivial conserved charges, there exist infinitely many of them, the first few are

$$(J_-)^2, \quad (J_-)^4, \quad (\partial_- J_-)^2, \quad \cdots \quad . \tag{22.52}$$

We do not analyze them further, just note that there is an infinite set of the charges which are in involution for the canonical Poisson bracket.

22.5.3 Conserved charges in the interacting theory

Now we want to extend the conserved charges to the interacting case defined by:

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - V(\varphi) = \partial_+\varphi\partial_-\varphi - V(\varphi) \quad \longrightarrow \quad \partial_+\partial_-\varphi = V'(\varphi). \tag{22.53}$$

The relevant change is that $J_- = \partial_-\varphi$ no longer depends on x_- only:

$$\partial_+ J_- = \partial_+\partial_-\varphi = V'(\varphi) \neq 0. \tag{22.54}$$

Our strategy is the following. We start with a nonzero conserved current component of the free theory, say $T_2 = (J_-)^2/2$, and try to extend it to a two-component current (T_2, Θ_0) which satisfies the conservation law

$$\partial_+ T_2 + \partial_- \Theta_0 = 0. \tag{22.55}$$

This is actually not a hard job since

$$\partial_+ T_2 = J_-\partial_+ J_- = J_- V'(\varphi) = \partial_- V(\varphi) \quad \longrightarrow \quad \Theta_0 = -V(\varphi). \tag{22.56}$$

After a similar calculation for $\bar{J}$ we can see that the resulting conserved charges are nothing but the light-cone components of the energy and momentum

$$Q_{\pm 1}[\varphi] = E[\varphi] \pm P[\varphi] = \int \left\{ \frac{1}{2}(\partial_\pm\varphi)^2 + V(\varphi) \right\} dx. \tag{22.57}$$

From their transformation rules under Lorentz transformation (22.10), $Q_{\pm 1} \to e^{\pm\Lambda} Q_{\pm 1}$, we conclude that they have spins ± 1.

At the level of spin 3, we need to combine the two quantities $(J_-)^4$ and $(\partial_- J_-)^2$ which cannot be conserved separately. Our tactic is the same as before. We are looking for conserved charges of the form

$$\left(T_4 = \frac{1}{4}(J_-)^4 + \alpha(\partial_- J_-)^2, \Theta_2\right) \quad \longrightarrow \quad \partial_+ T_4 + \partial_- \Theta_2 = 0. \tag{22.58}$$

Elementary calculation shows

$$\partial_+ T_4 = (J_-)^3 V' + 2\alpha J_-(\partial_- J_-)V'' = \partial_- \left[(J_-)^2 V\right] + 2J_-(\partial_- J_-)(\alpha V'' - V). \tag{22.59}$$

So a spin 3 conserved charge can exist provided that the potential satisfies the condition

$$V'' - \frac{1}{\alpha} V = 0 \quad \to \quad V = a\mathrm{e}^{\varphi/\sqrt{\alpha}} + b\mathrm{e}^{-\varphi/\sqrt{\alpha}}. \tag{22.60}$$

The corresponding integrable models are the sine-Gordon, sinh-Gordon and Liouville $(b = 0)$ theories. The current $\Theta_2 = -(J_-)^2 V$.

For the sine-Gordon theory, we obtain the following charges

$$Q_{\pm 3}[\varphi] = \int \mathrm{d}x \left\{ \frac{1}{2b^2}(\partial_\pm^2 \varphi)^2 - \frac{1}{8}(\partial_\pm \varphi)^4 + \frac{m^2}{b^2}(\partial_\pm \varphi)^2 (1 - \cos b\varphi) \right\}. \tag{22.61}$$

The existence of higher spin charges is very important. We will show in the quantum theory that higher spin charges will force the scattering matrix to factorize. By extending the present methodology one can construct higher spin charges in the sine-Gordon theory for each odd integer. Instead of following this route, we close the section by showing the existence of an infinite number of charges in an abstract way.

22.5.4 Integrability of the sine-Gordon theory

We start by introducing su(2) valued gauge potentials

$$A_x(\lambda) = \mathrm{i} \begin{pmatrix} \lambda & \frac{b}{2}\partial_+ \varphi \\ -\frac{b}{2}\partial_- \varphi & -\lambda \end{pmatrix}, \qquad A_t(\lambda) = \frac{1}{4\mathrm{i}\lambda} \begin{pmatrix} \cos b\varphi & -\mathrm{i}\sin b\varphi \\ \mathrm{i}\sin b\varphi & -\cos b\varphi \end{pmatrix}, \tag{22.62}$$

where, for simplicity, we use dimensionless coordinates: $x \to mx$, $t \to mt$. These matrices are non-abelian gauge potentials $A_\mu(x, t, \lambda)$ which define an su(2) valued field strength $F_{\mu\nu}$. The field strength vanishes,

$$F_{xt} = \partial_x A_t - \partial_t A_x + [A_x, A_t] = 0, \tag{22.63}$$

provided that φ satisfies the sine-Gordon equation of motion.

We define the quantity T as the solution of differential equations

$$\partial_\mu T(x, t, \lambda) = A_\mu(x, t, \lambda) T(x, t, \lambda), \qquad \mu = x, t. \tag{22.64}$$

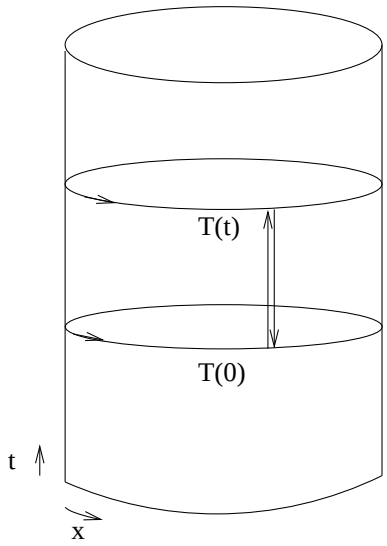


Fig. 22.5. Space-time cylinder with nontrivial integration contours for the $T(\lambda, t)$ matrices.

A representation is possible in terms of the path ordered exponential

$$T(x,t,\lambda) = \mathcal{P}\exp\left\{\int_{(x_0,t_0)}^{(x,t)} A_\mu(x,t)\mathrm{d}x^\mu\right\} \tag{22.65}$$

for a curve from the point (x_0, t_0) to (x, t). The usual choice of the curve is

$$T(x,t,\lambda) = \mathcal{T}\exp\left\{\int_{(x_0,t_0)}^{(x_0,t)} A_t(x_0,t')\mathrm{d}t'\right\}\mathcal{X}\exp\left\{\int_{(x_0,t)}^{(x,t)} A_x(x',t)\mathrm{d}x'\right\}, \tag{22.66}$$

where we introduced time and space orderings. Due to the vanishing of the field strength, $T(x,t,\lambda)$ does not depend on the path connecting the two points. Nevertheless it depends on the starting point. To avoid this deficiency, we consider the sine-Gordon theory with periodic boundary condition, when by surrounding the space circle with a loop at fixed time t the matrix T will depend only on t. One can show that the same quantity evaluated at time t' can be written as $T(\lambda,t') = GT(t,\lambda)G^{-1}$, where $G = \mathcal{T}\exp\left\{\int_{(x_0,t)}^{(x_0,t')} A_t(x_0,t'')\mathrm{d}t''\right\}$, see Fig. 22.5. As a consequence $\mathrm{Tr}T(\lambda,t)$ will be time independent, thus expanding this quantity in λ will generate an infinite number of conserved charges.

23 Conformal quantization

There are certain ambiguities in how to quantize an infinitely dimensional interacting system. Different approaches lead to different quantization schemes. Typically we split the system into a free part and a perturbation, which is supposed to be small. In the case of the sine-Gordon theory, there exist two choices for the free part. We can choose the free massless boson

$$\mathcal{L} = \mathcal{L}_0 - V(\varphi) = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - V(\varphi), \qquad V(\varphi) = 2\mu(1-\cos b\varphi), \quad (23.1)$$

where $\mu = m^2/(2b^2)$. In this case the perturbation is organized in powers of μ. Alternatively, instead of the mass we can send the coupling constant to zero: $b \to 0$. This decomposes the Lagrangian into the Klein-Gordon theory

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - \frac{m^2}{2}\varphi^2 - b^2U(\varphi), \quad U(\varphi) = \frac{m^2}{b^4}\sum_{n=2}^{\infty}\frac{(-1)^n b^{2n}}{(2n)!}\varphi^{2n} \quad (23.2)$$

and the perturbation $U(\varphi)$ has a power expansion in b. As the first step, the free theory is quantized and solved exactly and afterwards, the perturbation is taken into account. The perturbing operator is made to be well-defined by its normal ordering, what will change its parameters. As the solved free theories are different by the normal orderings, the parameters of the quantum theories will be different (scheme-dependent), too. Nevertheless, the physically measurable quantities have to coincide.

We present both approaches here since each has its own advantages. The first one is called the conformal quantization scheme. It proves to be useful in showing the quantum integrability of the model and that the perturbative expansion of its partition function can be mapped to that of the two-dimensional Coulomb gas. The second quantization scheme is the topic of Sect. 24. It is relevant in defining the scattering matrix and deriving its fundamental properties.

The conformal quantization scheme is established in this section. We first solve the free model which is the scale invariant/conformal theory [38, 39]. We analyze the theory on the space-time cylinder first, afterwards we map the system onto the conformal plane. Then we turn to the analysis of the perturbation. The perturbing operator will be a well-defined scaling field in the conformal field theory.

23.1 Massless free boson on the cylinder

We consider the free massless boson on both the cylinder and the full plane [39]. As the two cases have different canonical normalizations, we redefine the action on the cylinder as follows

$$S = \frac{g}{2}\int_{-\infty}^{\infty}\mathrm{d}t\int_0^L \mathrm{d}x\,\partial_\mu\Phi\partial^\mu\Phi, \qquad \eta = (+,-), \quad (23.3)$$

where we introduced a normalization parameter g and denoted the so-normalized field by Φ. (Thus for $g = 1$ we have $\Phi = \varphi$). As we intend to describe the sine-Gordon theory, the target space of the field is a circle of compactification radius $r = 1/b$. The periodic BC thus read

$$\Phi(L,t) = \Phi(0,t) + 2\pi r m, \qquad m \in \mathbb{Z}, \quad (23.4)$$

where the winding number m counts how many times the field winds around the space-time cylinder. It is a topological quantum number (soliton number in the perturbed theory) which is not changed by the continuous time evolution and labels different sectors of the quantum theory. In each sector, we expand the quantum field in Fourier components as

$$\Phi(x,t) = \Phi_0(t) + \frac{2\pi}{L} rmx + \sum_{n\neq 0} \Phi_n(t) \mathrm{e}^{\mathrm{i}2\pi x n/L}. \tag{23.5}$$

Not all components are independent. Since the field Φ is real, we have $\Phi_0^+ = \Phi_0$ and $\Phi_n^+ = \Phi_{-n}$. The orthogonality of the basis, $\int_0^L \mathrm{d}x\, \mathrm{e}^{\mathrm{i}2\pi x n/L} \mathrm{e}^{-\mathrm{i}2\pi x m/L} = L\delta_{n,m}$, can be used to write the Lagrangian in the form

$$L[\{\Phi_n, \dot\Phi_n\}] = \frac{Lg}{2} \sum_n \left(\dot\Phi_n \dot\Phi_{-n} - \frac{4\pi^2 n^2}{L^2} \Phi_n \Phi_{-n} \right) - \frac{Lg}{2} \left[\frac{4\pi^2 (rm)^2}{L^2} \right]. \tag{23.6}$$

The canonical momenta are defined in the standard way: $\pi_n = \partial L/\partial \dot\Phi_n = Lg\dot\Phi_{-n}$. The reality condition reads as $\pi_n^+ = \pi_{-n}$. The Hamiltonian $H = \sum \pi_n \dot\Phi_n - L$ takes the form

$$H = \frac{1}{2Lg} \sum_n \left(\pi_n \pi_{-n} + 4\pi^2 n^2 g^2 \Phi_n \Phi_{-n} \right) + \frac{Lg}{2} \left[\frac{4\pi^2 (rm)^2}{L^2} \right], \tag{23.7}$$

where the canonical commutation relations are $[\Phi_n, \pi_m] = \mathrm{i}\delta_{n,m}$. This shows that the Hamiltonian consists of independent harmonic oscillators with frequencies $\omega_n = 2\pi g|n|$. The $n = 0$ frequency vanishes and needs a special care (see below).

To diagonalize the Hamiltonian, we introduce the creation and annihilation operators

$$b_n = \frac{1}{\sqrt{2\omega_n}} (\omega_n \Phi_n + \mathrm{i}\pi_{-n}), \qquad [b_n, b_m^+] = \delta_{n,m}. \tag{23.8}$$

This would lead to the complete solution of the spectral problem. The massless boson is, however, very special. The eigenfunction of the wave equation can always be separated into a left and a right moving component. To respect this we introduce

$$a_n = \begin{cases} -\mathrm{i}\sqrt{n} b_n & \text{for } n > 0 \\ \mathrm{i}\sqrt{-n} b_{-n}^+ & \text{for } n < 0 \end{cases}, \qquad \bar a_n = \begin{cases} -\mathrm{i}\sqrt{n} b_{-n} & \text{for } n > 0 \\ \mathrm{i}\sqrt{-n} b_n^+ & \text{for } n < 0 \end{cases}, \tag{23.9}$$

where the inherited commutation relations take the factorized form

$$[a_n, a_m] = n\delta_{n+m}, \qquad [\bar a_n, \bar a_m] = n\delta_{n+m}, \qquad [\bar a_n, a_m] = 0. \tag{23.10}$$

The normal-ordered Hamiltonian[6]

$$H = \frac{2\pi}{L} \sum_{n>0} \left(a_{-n} a_n + \bar a_{-n} \bar a_n - \frac{c}{12} \right) + \frac{1}{2Lg} \pi_0^2 + \frac{Lg}{2} \left[\frac{4\pi^2 (rm)^2}{L^2} \right] \tag{23.11}$$

governs the time evolution of the various operators:

$$\dot\Phi_0 = \mathrm{i}[H, \Phi_0] = \frac{\pi_0}{Lg} \qquad \longrightarrow \qquad \Phi_0(t) = \Phi_0 + \frac{\pi_0}{gL} t, \tag{23.12}$$

[6] Here, c stands for a constant coming from the normal ordering, which will be later fixed to $c = 1$.

$$\dot{a}_n = \mathrm{i}[H, a_n] = -\mathrm{i}\frac{2\pi n}{L} a_n \qquad \longrightarrow \qquad a_n(t) = a_n \mathrm{e}^{-\mathrm{i}2\pi n t/L}. \tag{23.13}$$

The Hilbert space can be built up from the vacuum $|0\rangle$, defined by

$$a_n|0\rangle = 0, \qquad \bar{a}_n|0\rangle = 0, \qquad n > 0, \tag{23.14}$$

by the successive application of the creation operators a_{-n} and $\bar{a}_{-\bar{n}}$ as

$$a_{-n_1}^{k_1} \cdots a_{-n_N}^{k_N} \bar{a}_{-\bar{n}_1}^{\bar{k}_1} \cdots \bar{a}_{-\bar{n}_{\bar{N}}}^{\bar{k}_{\bar{N}}} |0\rangle. \tag{23.15}$$

The vacuum has vanishing winding $m = 0$ and momentum $\pi_0|0\rangle = 0$.

The movement of the zero mode Φ_0 is a free motion on the circle of radius r. Consequently the eigenvalues of π_0 can be n/r for any $n \in \mathbb{Z}$ not only for 0. Thus the full Hilbert space of the model contains states built over the ground-state of any sector

$$a_{-n_1}^{k_1} \cdots a_{-n_N}^{k_N} \bar{a}_{-\bar{n}_1}^{\bar{k}_1} \cdots \bar{a}_{-\bar{n}_{\bar{N}}}^{\bar{k}_{\bar{N}}} |n, m\rangle, \tag{23.16}$$

where the winding in this sector is m and the momentum of the zero mode is $\pi_0|n, m\rangle = (n/r)|n, m\rangle$. Clearly $\mathrm{e}^{\mathrm{i}\frac{n}{r}\Phi_0}$ generates $|n, m\rangle$ from the ground-state of the winding sector m. We can also introduce formally an operator M whose eigenvalue is m: $M|n, m\rangle = m|n, m\rangle$. In analogy with Φ_0, we also introduce its conjugate variable Ψ such that $[\Psi, M] = \mathrm{i}$ and $\mathrm{e}^{\mathrm{i}m\Psi}|n, 0\rangle = |n, m\rangle$. With these operators the energy eigenvalues can be calculated from

$$H = \frac{2\pi}{L} \sum_{n>0} \left(a_{-n} a_n + \bar{a}_{-n} \bar{a}_n - \frac{1}{12} \right) + \frac{2\pi}{L} \left[\frac{1}{4\pi g} \pi_0^2 + 4\pi g \left(\frac{rM}{2} \right)^2 \right]. \tag{23.17}$$

Putting back these expressions into $\Phi(x, t)$ yields the complete time evolution of the system:

$$\begin{aligned} \Phi(x,t) \quad &= \quad \Phi_0 + \frac{\pi_0}{gL} t + \frac{2\pi}{L} r M x \\ &\quad + \frac{\mathrm{i}}{\sqrt{4\pi g}} \sum_{n \neq 0} \frac{1}{n} \left(a_n \mathrm{e}^{\mathrm{i}\frac{2\pi}{L} n(x-t)} + \bar{a}_n \mathrm{e}^{-\mathrm{i}\frac{2\pi}{L} n(x+t)} \right) \end{aligned} \tag{23.18}$$

and solves the theory on the space-time cylinder. Notice that the formulas are simplified significantly for the choice $g = 1/(4\pi)$. There are further simplifications when we analyze the free theory on the complex plane.

23.2 Massless free boson on the complex plane

The complete solution of a quantum theory in general means the calculation of all correlation functions. It turns out that instead of working on the cylinder of circumference L it is advantageous to map the system onto the scaleless plane, where all formulas will simplify. To do so, we consider the Euclidean version of the theory by analytically continuing in the time variable $y = it$ and map the system via the exponential mapping to the plane, $x + iy = \xi \to z = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{L}\xi}$, as shown in Fig. 23.1. We also have $x - iy = \bar{\xi} \to \bar{z} = \mathrm{e}^{\mathrm{i}\frac{2\pi}{L}\bar{\xi}}$. As a consequence, the light-cone coordinates become the holomorphic and anti-holomorphic coordinates and we can use

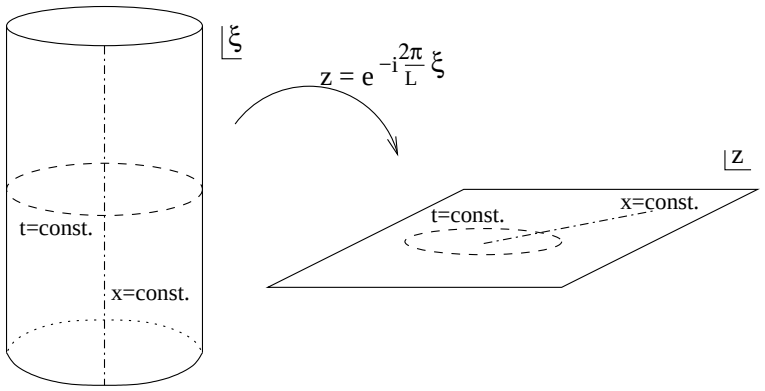


Fig. 23.1. Exponential mapping of the Euclidean space-time cylinder to the conformal plane. Equal time slices on the cylinder become concentric circles on the plane.

the powerful complex analysis. The left and right mover parts of the field $\Phi(z,\bar{z})$ give rise to holomorphic $\phi(z)$ and anti-holomorphic $\bar{\phi}(\bar{z})$ fields, $\Phi(z,\bar{z}) = \phi(z) + \bar{\phi}(\bar{z})$, where

$$\begin{aligned}
\phi(z) &= \frac{1}{\sqrt{4\pi g}}\left(\phi_0 - \mathrm{i}a_0 \ln z + \mathrm{i}\sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} a_n \frac{z^{-n}}{n}\right), \\
\bar{\phi}(\bar{z}) &= \frac{1}{\sqrt{4\pi g}}\left(\bar{\phi}_0 - \mathrm{i}\bar{a}_0 \ln \bar{z} + \mathrm{i}\sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \bar{a}_n \frac{\bar{z}^{-n}}{n}\right).
\end{aligned} \tag{23.19}$$

To have a compact notation we introduced the zero modes

$$\begin{aligned}
a_0 &= \frac{\pi_0}{\sqrt{4\pi g}} - \sqrt{4\pi g}\frac{rM}{2}, \qquad \bar{a}_0 = \frac{\pi_0}{\sqrt{4\pi g}} + \sqrt{4\pi g}\frac{rM}{2}, \\
\phi_0 &= \sqrt{4\pi g}\frac{\Phi_0}{2} - \frac{\Psi}{r\sqrt{4\pi g}}, \qquad \bar{\phi}_0 = \sqrt{4\pi g}\frac{\Phi_0}{2} + \frac{\Psi}{r\sqrt{4\pi g}},
\end{aligned} \tag{23.20}$$

such that the non-vanishing commutators are $[a_0,\phi_0] = [\bar{a}_0,\bar{\phi}_0] = -\mathrm{i}$. Considering these commutation relations, together with those in (23.10), we can calculate all correlation functions.

23.2.1 Operator Product Expansion

Products of operators are not well-defined in the quantum field theory. In order to define them properly, we need to introduce specific orderings. One of usual orderings is the time ordering, which on the plane leads to the radial ordering (see Fig. 23.1):

$$R(\phi(z_1)\phi(z_2)) = \begin{cases} \phi(z_1)\phi(z_2) & \text{if } |z_1| > |z_2|, \\ \phi(z_2)\phi(z_1) & \text{if } |z_2| > |z_1|. \end{cases} \tag{23.21}$$

Assuming that $|z_1| > |z_2|$ we can calculate the two-point function:

$$\begin{aligned}
&\langle 0|R(\phi(z_1)\phi(z_2))|0\rangle \\
&= \frac{1}{4\pi g}\langle 0|\left(-\mathrm{i}a_0\ln z_1 + \mathrm{i}\sum_{n>0} a_n\frac{z_1^{-n}}{n}\right)\left(\phi_0 + \mathrm{i}\sum_{n<0} a_n\frac{z_2^{-n}}{n}\right)|0\rangle \\
&= \frac{1}{4\pi g}\left[-\ln z_1 + \sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{z_2}{z_1}\right)^n\right] = \frac{-1}{4\pi g}\ln(z_1 - z_2). \qquad (23.22)
\end{aligned}$$

In the first step of the calculation, we omitted those operators which annihilate the vacuum. In the second step, in order to give meaning to the infinite sum, we took into account the radial ordering $|z_2|/|z_1| < 1$. Since we shall consider only well-defined products of operators, the radial ordering will not be written out explicitly; it will always be understood if no other indication is given. Combining the two chiral ϕ and $\bar{\phi}$ parts, we obtain the full correlation function:

$$\langle 0|\Phi(z_1,\bar{z}_1)\Phi(z_2,\bar{z}_2)|0\rangle = -\frac{1}{2\pi g}\ln(|z_1 - z_2|). \qquad (23.23)$$

We expect singular behavior whenever the operators are localized at the same space-time point $z_1 - z_2 = 0$. We face an infrared $z_1 - z_2 \to \infty$ singularity as well. This shows that Φ itself is not a well defined field. Indeed, in the Lagrangian of the sine-Gordon theory we have either the derivative of Φ or its exponential function.

Let us analyze the derivatives, the chiral currents

$$\begin{aligned}
J(z) &= \mathrm{i}\sqrt{4\pi g}\partial_z\phi(z) = \sum_n a_n z^{-n-1}, \\
\bar{J}(\bar{z}) &= \mathrm{i}\sqrt{4\pi g}\partial_{\bar{z}}\bar{\phi}(\bar{z}) = \sum_n \bar{a}_n \bar{z}^{-n-1}, \qquad (23.24)
\end{aligned}$$

which are conserved at the quantum level, too,

$$\bar{\partial}J(z) \equiv \partial_{\bar{z}}J(z) = 0, \qquad \partial\bar{J}(\bar{z}) \equiv \partial_z\bar{J}(\bar{z}) = 0. \qquad (23.25)$$

Their correlation function is easy to calculate. We either differentiate the expression (23.22) or directly use the definition

$$\langle 0|J(z)J(w)|0\rangle = \sum_{n>0,m<0} z^{-n-1}w^{-m-1}\langle 0|a_n a_m|0\rangle = z^{-2}\sum_{n=1}^{\infty} n\left(\frac{w}{z}\right)^{n-1}. \qquad (23.26)$$

It stands to reason that the radial ordering makes the series convergent for $|z| > |w|$. This function then can be analytically continued to a single valued correlator

$$\langle 0|J(z)J(w)|0\rangle = \frac{1}{(z-w)^2}. \qquad (23.27)$$

We can introduce another well-defined product of operators, namely the normal ordered product

$$:J(z)J(w):, \qquad :a_n a_m: = \begin{cases} a_n a_m & \text{if } m > 0, \\ a_m a_n & \text{otherwise,} \end{cases} \qquad (23.28)$$

where the normal ordering means that the annihilation operators $\{a_m, m > 0\}$ are put on the right of the creation operators. We can decompose the field into positive and non-negative modes, so that $J(z) = J_>(z) + J_\leq(z)$. In this notation, the normal ordering is simply $: J(z)J(w) := J_\leq(z)J(w) + J(w)J_>(z)$. Its advantage consists in the fact that it is nonsingular at $z = w$, where it defines a well-behaving operator. Using that $[J_>(z), J(w)] = 1/(z-w)^2$ we can express the radially ordered product in terms of the normal ordered product and the vacuum expectation value:

$$J(z)J(w) = \frac{1}{(z-w)^2} + : J(z)J(w) : . \tag{23.29}$$

This is the Wick theorem.

There is an important notion in quantum field theory, the so-called operator product expansion (OPE). It expresses the fact that there is a basis of well-defined local operators and every product of local operators can be expressed in terms of this basis. In particular, in the previous case we can write

$$\begin{aligned} J(z)J(w) &= \frac{1}{(z-w)^2} + : J(w)J(w) : + (z-w) : J(w)\partial_w J(w) : + \cdots \\ &\quad + (z-w)^k \frac{1}{k!} : J(w)\partial_w^k J(w) : + \cdots . \end{aligned} \tag{23.30}$$

The general case has the following structure

$$\mathcal{O}_i(z)\mathcal{O}_j(w) = \sum_k C_{ij}^k (z-w)^k \mathcal{O}_k(w), \tag{23.31}$$

where only a finite number of negative exponents are present. In this expansion all fields have a definite scaling dimension.

23.2.2 Conformal transformations

The free massless boson is conformally invariant. This can be seen by calculating its energy momentum tensor

$$T_{\mu\nu} = g\partial_\mu\Phi\partial_\nu\Phi - \frac{g}{2}\eta_{\mu\nu}\partial_\mu\Phi\partial^\mu\Phi \tag{23.32}$$

and observing that it is traceless: $T_\mu^\mu \equiv T_{00} - T_{11} = 0$. Indeed, according to Noether's theorem, the coordinate transformation $x^\mu \to x^\mu + \delta x^\mu$ is a symmetry if and only if the current $j_\mu = T_{\mu\nu}\delta x^\nu$ is conserved, $\partial^\mu j_\mu = 0$. Thus the scale transformation $\delta x^\mu = \epsilon x^\mu$ is a continuous symmetry. Since the stress tensor is also symmetric, $T_{10} = T_{01}$, it has a factorizing form in light-cone coordinates: $T_{+-} = T_{-+} = 0$ and $T_{\pm\pm} = T_{00} \pm (T_{01} + T_{10}) + T_{11}$.

Expressing the energy momentum tensor on the Euclidean plane in holomorphic and anti-holomorphic coordinates, the two nontrivial elements are $T_{zz} \equiv T(z)$ and $T_{\bar z\bar z} \equiv \bar T(\bar z)$. They can be expressed in terms of the conserved chiral current as follows

$$\begin{aligned} T(z) &= \frac{1}{2} : J(z)J(z) := \sum_n L_n z^{-n-2}, \\ \bar T(\bar z) &= \frac{1}{2} : \bar J(\bar z)\bar J(\bar z) := \sum_n \bar L_n \bar z^{-n-2}. \end{aligned} \tag{23.33}$$

The modes read as $L_n = \frac{1}{2}\sum_m :a_m a_{n-m}:$, $L_0 = \sum_{n>0} a_{-n}a_n + \frac{1}{2}a_0^2$. Together with $\bar{L}_n$, they form the symmetry algebra of the model, which is two commuting copies of the algebra

$$[L_n, L_m] = (n-m)L_{n+m} + \frac{c}{12}n(n^2-1)\delta_{n+m} \tag{23.34}$$

with $c = 1$. This algebra is called the Virasoro algebra and c is called its central charge. This is the quantum version of the conformal symmetry algebra.

The conformal transformation on the plane can be written as two independent $z \to f(z)$ and $\bar{z} \to \bar{f}(\bar{z})$ conformal transformations, and conservation of the energy momentum tensor follows from this symmetry: $\partial_{\bar{z}} T(z) = \partial_z \bar{T}(\bar{z}) = 0$. Due to Noether's theorem, the infinitesimal version of the conformal transformation $z \to z + \epsilon(z)$ is generated by the conserved charge

$$Q = \oint \frac{\mathrm{d}z}{2\pi\mathrm{i}} T(z)\epsilon(z) \tag{23.35}$$

itself; the integral is over the circle $|z| = \mathrm{const.}$ which is the image of the equal-time slice under the exponential map. This charge implements the coordinate transformation $z \to z + \epsilon(z)$ on the fields by the equal-time commutator. Since the order of the operators can be encoded into the relative absolute value of their arguments, we can write

$$\begin{aligned} \delta_\epsilon \mathcal{O}(w) &= [Q, \mathcal{O}(w)] = \frac{1}{2\pi\mathrm{i}} \left(\oint_{|z|>|w|} - \oint_{|z|<|w|} \right) \mathrm{d}z\, \epsilon(z) T(z)\mathcal{O}(w) \\ &= \frac{1}{2\pi\mathrm{i}} \oint_w \mathrm{d}z\, \epsilon(z) T(z)\mathcal{O}(w), \end{aligned} \tag{23.36}$$

where the radial ordering is understood everywhere. In the last equation, we deformed the contour to enclose w as the operator product is singular only for $z \to w$. Note that the integration picks up only the singular terms of the OPE by residue theorem (23.31). We spell out the meaning of these formulas. We can calculate the singular parts of $T(z)$ and $J(w)$ by using

$$T(z)J(w) = \frac{J(w)}{(z-w)^2} + \frac{\partial_w J(w)}{(z-w)} + O(1), \tag{23.37}$$

where we used that $2T(z) = [J_>(z) + J_\leq(z)]J_>(z) + J_\leq(z)[J_>(z) + J_\leq(z)]$ and rewrote the radially ordered expression in terms of contractions (commutators) and nonsingular normal ordered expression. Plugging back this expression into (23.36) and performing the integration, we obtain the transformation of the field $J(w)$ under an infinitesimal conformal transformation $z \to z + \epsilon(z)$:

$$\delta_\epsilon J(z) = [\partial_z \epsilon(z)]J(z) + \epsilon(z)\partial_z J(z). \tag{23.38}$$

This is equivalent to (23.24) and the transformation of the scalar field $\delta_\epsilon \phi(z) \equiv \phi(z + \epsilon(z)) - \phi(z) = \epsilon(z)\partial_z \phi(z)$. By iterating the infinitesimal transformation, the field $J(z)$ changes under the conformal transformation $z \to w(z)$ as follows

$$J(z) = \left(\frac{\partial w}{\partial z}\right)^h J(w(z)), \qquad h = 1. \tag{23.39}$$

Fields which transform themselves in this way for generic h are called primary fields of weight h. Thus $J(w)$ is a primary field of weight 1. There are other primary fields in the theory which are investigated in the next part.

Finally we note that not all fields are primary fields. Consider the energy momentum tensor $T(z)$ as an example. One can easily check that

$$T(z)T(w) = \frac{c}{2(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial_w T(w)}{(z-w)} + O(1). \tag{23.40}$$

This means that for "large" conformal transformations $z \to w(z)$ we have

$$T(z) \to (\partial_z w)^2 T(w) + \frac{c}{12}\frac{\partial_z w \partial_z^3 w - 3(\partial_z^2 w)^2/2}{(\partial_z w)^2}. \tag{23.41}$$

In particular, this means that if we normalize the vacuum energy to zero on the plane, $\langle T(z)\rangle = 0$, then on the cylinder $z = \exp(\mathrm{i}2\pi\xi/L)$ we have $\langle T(\xi)\rangle = -c/24$. Repeating the same calculations for $\bar{T}(\bar{z})$ and taking into account the normalization of the energy, we obtain the normal-ordering contribution $-c/12$ in (23.11), as was promised.

23.2.3 Primary fields

Recall that the scalar field itself is not a well-defined operator as its pair correlation functions contain logarithms. In the action of the sine-Gordon theory, we have either its derivatives or exponentials. We have already analyzed the derivatives of the scalar field. Now intend to analyze the operators

$$V_{(n,m)}(z,\bar{z}) = :\mathrm{e}^{\mathrm{i}\frac{n}{r}\Phi(z,\bar{z})+\mathrm{i}\frac{mr}{2}4\pi g\tilde{\Phi}(z,\bar{z})}:= :e^{\mathrm{i}q\phi(z)+\mathrm{i}\bar{q}\bar{\phi}(\bar{z})}: . \tag{23.42}$$

Here, we apply the parameterization (n,m) and $(q,\bar{q})$ in parallel, the connection between them follows from the definitions

$$\Phi(z,\bar{z}) = \phi(z) + \bar{\phi}(\bar{z}), \qquad \tilde{\Phi}(z,\bar{z}) = \phi(z) - \bar{\phi}(\bar{z}), \tag{23.43}$$

so that $q+\bar{q} = 2n/r$ and $q-\bar{q} = 4\pi g m r$. The singular part of the OPE can be calculated by commuting the positive modes to the right:

$$J(z)V_{(n,m)}(w,\bar{w}) = [J_>(z), V_{(n,m)}(w,\bar{w})] = \frac{q}{4\pi g}\frac{V_{(n,m)}(w,\bar{w})}{z-w} + \cdots, \tag{23.44}$$

$$T(z)V_{(n,m)}(w,\bar{w}) = \frac{q^2}{8\pi g}\frac{V_{(n,m)}(w,\bar{w})}{(z-w)^2} + \frac{\partial_w V_{(n,m)}(w,\bar{w})}{(z-w)} + \cdots. \tag{23.45}$$

Similar formulas hold for the anti-holomorphic quantities. We see that $V_{(n,m)}(z,\bar{z})$ is a primary field of conformal weights $h_{(n,m)} = q^2/(8\pi g)$ and $\bar{h}_{(n,m)} = \bar{q}^2/(8\pi g)$ with respect to the conformal energy momentum tensor. This field is transformed for the $z \to z+\epsilon(z)$ infinitesimal conformal transformation as

$$\delta_\epsilon V_{(n,m)}(z,\bar{z}) = hV_{(n,m)}(z,\bar{z})\partial_z\epsilon + \epsilon\partial_z V_{(n,m)}(z,\bar{z}). \tag{23.46}$$

If we exponentiate this transformation to a large $z \to w(z)$, $\bar{z} \to \bar{w}(\bar{z})$ conformal transformation, the field will change as

$$V(z,\bar{z}) = \left(\frac{\partial w}{\partial z}\right)^{h} \left(\frac{\partial \bar{w}}{\partial \bar{z}}\right)^{\bar{h}} V(w,\bar{w}), \tag{23.47}$$

where we assumed that the anti-holomorphic transformations go in parallel with the holomorphic ones.

There is an interesting phenomenon in conformal theories: The local operators of the theory are in one-to-one correspondence with the Hilbert space of the model. In the present case, if we act with $V_{(n,m)}(z,\bar{z})$ on the vacuum and send the arguments to zero, we find

$$|n,m\rangle = \lim_{z,\bar{z}\to 0} V_{(n,m)}(z,\bar{z})|0\rangle. \tag{23.48}$$

The fields which correspond to $a_{-k-1}|n,m\rangle$ are proportional to $: (\partial^k J)V_{(n,m)} :$. Applying iteratively this observation, we can generate all fields for any state. In particular $V_{(0,0)}$ is the identity operator.

As the field Φ involves uncoupled harmonic oscillators a_n, the commutator of a positive mode with a negative mode is not an operator any more: $\mathrm{e}^{a_n}\mathrm{e}^{a_{-n}} = \mathrm{e}^{a_{-n}}\mathrm{e}^{a_n}\mathrm{e}^{[a_n,a_{-n}]}$. This implies the relation

$$V_{(q,\bar{q})}(z,\bar{z})V_{(q',\bar{q}')}(w,\bar{w}) = (z-w)^{\frac{qq'}{4\pi g}}(\bar{z}-\bar{w})^{\frac{\bar{q}\bar{q}'}{4\pi g}} : V_{(q,\bar{q})}(z,\bar{z})V_{(q',\bar{q}')}(w,\bar{w}) : . \tag{23.49}$$

Applying successively the same trick we can calculate all correlators of primary fields:

$$\begin{aligned}\langle 0|V_{(q_1,\bar{q}_1)}(z_1,\bar{z}_1)\cdots V_{(q_N,\bar{q}_N)}(z_N,\bar{z}_N)|0\rangle &= \delta(\sum_i q_i)\delta(\sum_i \bar{q}_i) \\ &\times \prod_{i<j}(z_i-z_j)^{\frac{q_i q_j}{4\pi g}} \prod_{i<j}(\bar{z}_i-\bar{z}_j)^{\frac{\bar{q}_i\bar{q}_j}{4\pi g}},\end{aligned} \tag{23.50}$$

where $\delta(\sum_i q_i) = 1$ if the total charge vanishes, $\sum_i q_i = 0$, and zero otherwise. The charge conservation comes from the fact that only the identity operator has non-vanishing vacuum expectation value.

Without making any relation to the already calculated spectrum of states $n, m \in \mathbb{Z}$, we could leave the spectrum of q's unknown and calculate just the correlation functions (23.50). Demanding these correlation functions to be single valued leaves two choices for the allowed (n,m) pairs. The first choice $n \in \mathbb{Z}$, $m \in \mathbb{Z}$ is the subject of this work. The other choice $(n \in \mathbb{Z}, m \in 2\mathbb{Z}) \cup \left(n \in \mathbb{Z} + \frac{1}{2}, m \in 2\mathbb{Z}+1\right)$ corresponds to the Thirring model of interacting fermion fields.

23.3 Perturbation of the massless free boson: sine-Gordon theory

We can define the sine-Gordon theory on the space-time cylinder as a perturbation of the already solved massless free boson (conformal field) theory, say with $g = 1$:

$$\mathcal{L} = \mathcal{L}_0 - \mu : \cos b\varphi := \frac{1}{2}\left[(\partial_t\Phi)^2 - (\partial_x\Phi)^2\right] - \mu\left[V_{(1,0)} + V_{(-1,0)}\right], \tag{23.51}$$

where we used the already well-defined operators $V_{(\pm 1,0)} =: \mathrm{e}^{\pm \mathrm{i}\frac{1}{r}\Phi(x,t)} :$. The Hamiltonian of the sine-Gordon model can be expressed as

$$H = H_0 + \mu \int_0^L \mathrm{d}x \left[V_{(1,0)}(x,t) + V_{(-1,0)}(x,t) \right], \tag{23.52}$$

where the unperturbed, conformal Hamiltonian is

$$H_0 = \frac{2\pi}{L} \left[L_0 + \bar{L}_0 - \frac{1}{12} \right]. \tag{23.53}$$

To be able to calculate its matrix elements, we map the perturbation operators by the conformal transformation, shown in Fig. 23.1, onto the plane. As the perturbation is a primary field, we have

$$V(x,t) = V(\xi,\bar{\xi}) = V(z,\bar{z}) \left(\frac{\mathrm{d}z}{\mathrm{d}\xi} \right)^h \left(\frac{\mathrm{d}\bar{z}}{\mathrm{d}\bar{\xi}} \right)^{\bar{h}} = V(z,\bar{z}) \left(-\frac{2\pi \mathrm{i}}{L} z \right)^h \left(\frac{2\pi \mathrm{i}}{L} \bar{z} \right)^{\bar{h}}. \tag{23.54}$$

In polar (r,θ)-coordinates, $z = r\mathrm{e}^{\mathrm{i}\theta}$ and $\bar{z} = r\mathrm{e}^{-\mathrm{i}\theta}$, the Hamiltonian takes the form

$$\begin{aligned} H &= \frac{2\pi}{L} \Bigg\{ L_0 + \bar{L}_0 - \frac{1}{12} \\ &\quad + \mu \left(\frac{2\pi}{L} \right)^{2(h-1)} 2\pi \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \left[V_{(1,0)}(\mathrm{e}^{\mathrm{i}\theta}, \mathrm{e}^{-\mathrm{i}\theta}) + V_{(-1,0)}(\mathrm{e}^{i\theta}, \mathrm{e}^{-i\theta}) \right] \Bigg\}. \end{aligned} \tag{23.55}$$

The perturbation can be classified by its behaviour for large L. If the perturbation gets stronger ($h < 1$) it is "relevant", if the perturbation gets weaker ($h > 1$) it is "irrelevant", while for $h = 1$ it is "marginal". An analogous classification of the perturbations can be formulated in terms of the dimension of the coupling constant. The dimension of the energy is 1, $[H] = 1$, the dimension of the volume is -1, $[L] = -1$, so the coupling has dimension $[\mu] = 2(1-h)$.

An obvious way to calculate the spectrum of the sine-Gordon theory is to use the Hamiltonian perturbation theory. The result is an expansion of the energy in powers of μ, which is related by dimensional arguments to an expansion in $L^{2(1-h)}$:

$$E_n(L) = \frac{2\pi}{L} \left[E_{|n\rangle} - \frac{1}{12} + \sum_k c_k (\mu)^k \left(\frac{2\pi}{L} \right)^{2k(h-1)} \right], \tag{23.56}$$

where $E_{|n\rangle}$ is the conformal energy of the unperturbed state $|n\rangle$ and the coefficients c_k can be calculated from the matrix elements of the perturbing operator. Evidently,

$$c_1 = 2\pi \langle n | \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} \left[V_{(1,0)}(\mathrm{e}^{\mathrm{i}\theta}, \mathrm{e}^{-\mathrm{i}\theta}) + V_{(-1,0)}(\mathrm{e}^{\mathrm{i}\theta}, \mathrm{e}^{-\mathrm{i}\theta}) \right] |n\rangle = 0. \tag{23.57}$$

As concerns the ground-state, we can obtain formulas based on the perturbative expansion of the partition function which are easier to evaluate.

There is another standard way of calculating the spectrum in quantum theory. The idea is to take the energy levels of the unperturbed theory below certain energy level and use their linear combination in the variational method. This can be shown to be equivalent to diagonalize the

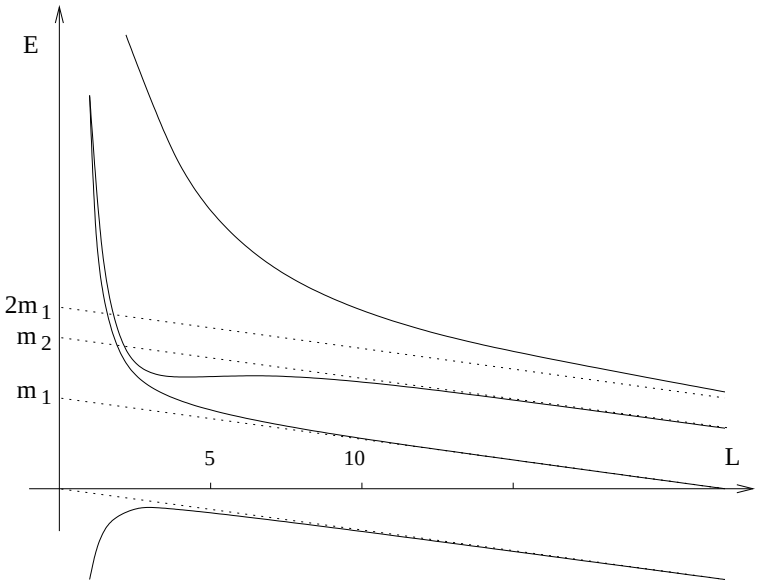


Fig. 23.2. Schematic numerical spectrum of the sine-Gordon theory in a finite volume.

interacting Hamiltonian on the truncated Hilbert space. This method is called the truncated conformal space approach (TCSA) [40, 41]. A typical numerical spectrum of the sine-Gordon theory obtained in this way is show in Figure 23.2. All energy levels for large volume behave as

$$E_n(L) = E_n(\infty) - e_0 L + O\left(\mathrm{e}^{-mL}\right), \tag{23.58}$$

where e_0 is the bulk $(L \to \infty)$ ground-state energy density. By analyzing the numerical results for $E_n(\infty)$, we can read off the masses of the excitations, which have to correspond to the quantized versions of the soliton, the anti-soliton and, in a certain parameter range, to their boundstates – the breathers.

23.3.1 Conserved charges

Now we analyze how the classical higher-spin charges can survive the quantization [42, 43]. We follow the same tactic as we did at the classical level: We try to find such deformations of the critical conformal (unperturbed $\mu = 0$) theory to an off-critical ($\mu \neq 0$) theory which preserve conservation laws. In the critical case, any differential polynomials of the current J is conserved,

$$\bar{\partial} A(z) = 0, \qquad A(z) =: \partial^{n_1} J(z) \cdots \partial^{n_N} J(z) : \tag{23.59}$$

and similarly for $\bar{A}(\bar{z})$. This equation is an operator equation which is understood in a weak sense: it is valid for the correlator of $A(z)$ with any operator $\mathcal{O}$. We are interested in higher-spin

conserved charges, so we keep only those differential polynomials which are not total derivatives themselves. Just as in the classical case, the first few read as

$$: J(z)^2 :, \qquad : J(z)^3 :, \qquad : J(z)^4 :, \qquad : (\partial J(z))^2 : . \tag{23.60}$$

Let us study first how the conservations are deformed off-critically, i.e. how $A(z)$ acquires a $\bar{z}$-dependence when $\mu \neq 0$. We analyze a generic correlation function of $A(z)$ and differentiate it with respect to $\bar{z}$:

$$\begin{aligned} \bar{\partial}\langle A(z)\mathcal{O}\rangle &= \bar{\partial}\frac{\int [\mathrm{d}\Phi]\mathrm{e}^{-S_0-\mu S_I}A(z)\mathcal{O}}{\int [\mathrm{d}\Phi]\mathrm{e}^{-S_0-\mu S_I}} = \bar{\partial}\frac{\int [\mathrm{d}\Phi]\mathrm{e}^{-S_0}\mathrm{e}^{-\mu S_I}A(z)\mathcal{O}}{\int [\mathrm{d}\Phi]\mathrm{e}^{-S_0}\mathrm{e}^{-\mu S_I}} \\ &= \bar{\partial}\langle \mathrm{e}^{-\mu S_I}A(z)\mathcal{O}\rangle_c = \bar{\partial}\sum_{n=1}^{\infty}\frac{\mu^n}{n!}\langle (-S_I)^n A(z)\mathcal{O}\rangle_c . \end{aligned} \tag{23.61}$$

Here, $\langle\rangle_c$ denotes the connected correlator of the critical theory; disconnected diagrams in the perturbative evaluation of the numerator are canceled by the corresponding terms from the denominator. Since Eq. (23.61) is valid for any operator $\mathcal{O}$ we can extract the operator equation

$$\bar{\partial}A(z) = \bar{\partial}\sum_n \frac{\mu^n}{n!}(-S_I)^n A(z), \tag{23.62}$$

where the rhs is a perturbative expansion in the coupling constant. Let us focus on the first order term

$$\bar{\partial}A(z) = \mu\bar{\partial}\int \mathrm{d}w\mathrm{d}\bar{w}\, V(w,\bar{w})A(z) + O(\mu^2). \tag{23.63}$$

The $\bar{z}$ dependence of the integral comes from the singular behavior of the OPE

$$A(z)V(w,\bar{w}) = \frac{\mathcal{O}^{AV}_{-k}}{(z-w)^k} + \cdots + \frac{\mathcal{O}^{AV}_{-1}}{(z-w)} + \text{regular terms.} \tag{23.64}$$

To evaluate the integral, we introduce the coordinates $w = z + r\mathrm{e}^{\mathrm{i}\phi}, \bar{w} = \bar{z} + r\mathrm{e}^{-\mathrm{i}\phi}$ and integrate over $\int_\epsilon^\infty r\mathrm{d}r \int_0^{2\pi}\mathrm{d}\phi$. To avoid the singularity of the integrand, we have introduced a regularization parameter ϵ. This can be implemented by introducing into the integrand the step function $\theta(r^2-\epsilon^2) = \theta((z-w)(\bar{z}-\bar{w})-\epsilon^2)$. This regulator is the only function of $\bar{z}$ in the integrand. Since

$$\bar{\partial}\theta((z-w)(\bar{z}-\bar{w})-\epsilon^2) = (z-w)\delta^{(2)}(|z-w|^2), \tag{23.65}$$

the only non-vanishing contribution to the integral comes from the $\mathcal{O}^{\Lambda V}_{-1}$ term:

$$\bar{\partial}A(z) = \mu\mathcal{O}^{AV}_{-1} + O(\mu^2). \tag{23.66}$$

The first order perturbative correction is exact in most cases. This can be seen by analyzing the dimensions of each term in the perturbative expansion

$$\bar{\partial}A(z) = \mu\mathcal{O}_1 + \mu^2\mathcal{O}_2 + \cdots + \mu^n\mathcal{O}_n + \cdots . \tag{23.67}$$

level of A	non-derivative operators	level of $\mathcal{O}_{-1}^{AV}$	derivative operators	non-derivative operators
1	-	0	-	V
2	J^2	1	∂V	-
3	J^3	2	$\partial^2 V$	J^2V
4	J^4 ;$(\partial J)^2$	3	$\partial^3 V; \partial(J^2V)$	J^3V

Tab. 23.1. The list of the operators at the first few levels, both the critical conserved currents, A, and its possible counterparts $\mathcal{O}_{-1}^{AV}$. In representing the operators we used that $\partial V \propto JV$.

If the dimension of A is $(s,0)$ then in the n^{th}-order term we must have

$$(s,1) = \left(n(1-h) + h_{\mathcal{O}_n}, n(1-h) + \bar{h}_{\mathcal{O}_n}\right). \tag{23.68}$$

Clearly for $n=1$ we have a solution in terms of $\mathcal{O}_1 \propto \mathcal{O}_{-1}^{AV}$ whose dimension is $(h+s-1,h)$. For a generic irrational b^2 in the sine-Gordon theory, however, we cannot have solutions for other $n>1$.

To summarize, we found that at any order of the perturbation theory the conservation law gets deformed as

$$\bar{\partial} A(z) = \mu \mathcal{O}_{-1}^{AV}. \tag{23.69}$$

This will lead to an off-critical conserved charge only if $\mathcal{O}_{-1}^{AV}$ is a total derivative: $\mathcal{O}_{-1}^{AV} = \partial B$. Our job is to find such A's which satisfy this requirement. To show the existence of the conserved charges, it is sufficient to compare the dimensions of the A and AV spaces at s and $s-1$ levels. This argument is called the counting argument [42, 43]. The explicit form of the operators for the first few s are shown in Table 23.3.1. The operator $\bar{\partial}$ in Eq. (23.69) is a horizontal map. This means that J^2 is mapped onto ∂V which is a total derivative, thus J^2 as a conserved current has an off-critical integrable deformation. This is not a surprise as it corresponds to the off-critical energy momentum tensor. The current J^3 is mapped also to non-derivative J^2V, so it is not conserved. But at level four, since the space of non derivative operators is only one-dimensional, we can always take such a combination of J^4 and $(\partial J)^2$ that the result is a total derivative. Thus we can deduce the existence of a conserved current just by comparing the dimensions of the spaces.

One can show that there is an infinite number of conserved charges, so the sine-Gordon theory is integrable at the quantum level, too.

24 Lagrangian quantization

In this section, we quantize (preferentially) the sinh-Gordon theory in the Lagrangian framework. We consider this theory as the perturbation of the free massive boson (Klein-Gordon model), which is quantized first. The potential is treated perturbatively, it is supposed to be weak in the sense that the particle spectrum of the free model is not changed. This assumption is valid for the sinh-Gordon theory, where the only particle exist already in the Klein-Gordon model. In the sine-Gordon case, however, additionally to the breather type solution, which is the analogue of the sinh-Gordon particle, there are non-perturbative particles like the soliton and the anti-soliton. Nevertheless, our approach is based on general field theoretical investigations and the conceptual consequences are valid for any theory of quantum particles, even for the quantum counterparts of the soliton and anti-soliton.

We start the section by introducing the quantum analogue of the classical time shift, the scattering phase. We show how they are related in the semi-classical limit, which makes a bridge between the classical and quantum descriptions [44]. Then we turn to the quantization of the sinh-Gordon theory in the perturbative scheme: The free Klein-Gordon part is quantized first and then the interaction is taken into account in the interaction picture. We introduce the notion of asymptotic states and their scattering (S) matrix. Reduction formula links the S-matrix to the correlation functions. It makes possible to derive the crossing symmetry of the S-matrix and analyze its analytical structure [45].

24.1 Semi-classical considerations, phase shifts

We recall that the soliton and the anti-soliton are treated as particles. The soliton feels the anti-soliton as an attractive potential and so experiences a time shift when passing by it. We express this time shift in a form which can be linked easily to the quantum description.

Let us consider a classical particle of mass m moving in a localized potential $V(x)$, see Fig. 24.1. The time shift is defined by comparing the motion in the potential to the free motion,

$$\Delta t = (t_{\rm final} - t_{\rm initial})\Big|_V - (t_{\rm final} - t_{\rm initial})\Big|_{\rm free}. \tag{24.1}$$

The difference between the initial and final times can be computed as

$$t_f - t_i = \int_{x_i}^{x_f} \frac{{\rm d}x}{v(x)} = \int_{x_i}^{x_f} \frac{\partial p(x,E)}{\partial E}{\rm d}x, \qquad p(x,E) = \sqrt{2m[E-V(x)]}, \tag{24.2}$$

where $v(x)$ is the space-dependent velocity and we used the Hamilton equation of motion $v(x) =$

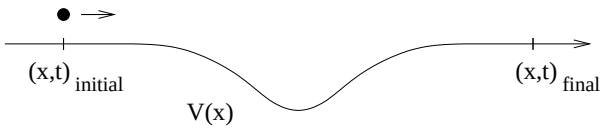


Fig. 24.1. Particle moves in a localized potential.

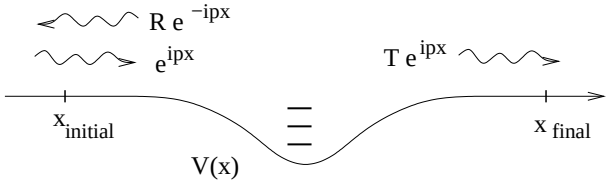


Fig. 24.2. Quantum mechanical wave function in a localized potential. In the asymptotic regions we have plane waves, while in the central region we might have boundstates. All information is contained in the reflection and transmission coefficients.

$\frac{\partial H}{\partial p}(x)$. Thus for a given energy E the time shift is

$$\Delta t(E) = \partial_E \int_{x_i}^{x_f} [p(x,E) - p(E)]\,\mathrm{d}x. \tag{24.3}$$

This is the quantity which we would like to link to the quantum mechanical phase shift.

Let us now study the quantum mechanics of the particle in the same potential, see Fig. 24.2. Since at large negative and positive x the potential vanishes, we have plane wave solutions there and the information on the potential is contained in the reflection and transmission coefficients. Notice that at the quantum level we may have the reflection as well as a discrete set of bound-states. The effect of the interaction when the particle passed through the potential is in the transmission coefficient $T = \exp(\mathrm{i}2\delta)$, or the phase-shift δ. In order to make a link to the classical description, we calculate the transmission coefficient in the semi-classical approximation $\hbar \to 0$. That is we solve the Schrödinger equation by separating the amplitude and the phase as

$$\hat{H}(\hat{p},x)\Psi(x) = E\Psi(x), \qquad \Psi(x,t) = A(x,t)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(x,t)}, \tag{24.4}$$

where it is supposed that the wave function oscillates quickly, $S(x,t) \gg \hbar$. (We use $\hbar = 1$ from now on). By expanding the Schrödinger equation (24.4) in $\hbar$ one can show that $S(x,t)$ is the classical action

$$S(x,t) = \int_{x_i}^{x} p(x',E)\mathrm{d}x' + \mathrm{const}. \tag{24.5}$$

The phase shift can be obtained from T by comparing to the free propagation:

$$2\delta(E) = \int_{x_i}^{x_f} [p(x,E) - p(E)]\,\mathrm{d}x. \tag{24.6}$$

Comparing the phase shift (24.6) to the classical time shift (24.3) we conclude that, in the semi-classical approximation,

$$\partial_E \delta(E) = \frac{1}{2}\Delta t(E). \tag{24.7}$$

We can integrate this equation from the threshold energy of the scattering solutions:

$$\delta(E) = \delta(E_{th}) + \frac{1}{2}\int_{E_{th}}^{E} \Delta t(E')\mathrm{d}E' = n_B\pi + \frac{1}{2}\int_{E_{th}}^{E} \Delta t(E')\mathrm{d}E', \tag{24.8}$$

where n_B is the number of boundstates in the semi-classical approximation.

We expect that an analogous formula will be valid for the field theory as well [44]. Thus to make correspondence to time shifts of Section 1, we need to introduce and calculate the scattering matrix, which is the field theoretical analogue of the transmission factor.

24.2 Quantization based on the Klein-Gordon theory

Referring to our previous discussion, we decompose the sinh-Gordon theory into the free and interaction parts as follows

$$\mathcal{L} = \frac{1}{2}(\partial_t\varphi)^2 - \frac{1}{2}(\partial_x\varphi)^2 - \frac{m^2}{2}\varphi^2 - b^2U(\varphi), \qquad U(\varphi) = \frac{m^2}{b^4}\sum_{n=2}^{\infty}\frac{b^{2n}}{(2n)!}\varphi^{2n}. \tag{24.9}$$

The free part can be obtained for $b = 0$,

$$\mathcal{L}_0 = \frac{1}{2}(\partial_t\varphi_0)^2 - \frac{1}{2}(\partial_x\varphi_0)^2 - \frac{m^2}{2}\varphi_0^2, \tag{24.10}$$

where the free nature of the field is emphasized by the notation φ_0. First we quantize the free part and subsequently define the sinh-Gordon QFT in the interaction picture.

24.2.1 Solving the free part

It is easy to quantize the free massive boson. We proceed in a similar way we solved the massless free boson in the previous section, but now we work on an infinite line. We define the conjugate momenta to the field φ_0 and require that only equal-time commutation relations are nonzero:

$$\frac{\delta\mathcal{L}_0}{\delta(\partial_t\varphi_0)} = \pi = \partial_t\varphi_0, \qquad [\pi(x,t), \varphi_0(x',t)] = -\mathrm{i}\delta(x-x'). \tag{24.11}$$

The Hamiltonian is obtained via the Legendre transformation by integrating $\pi(\partial_t\varphi_0) - \mathcal{L}_0$,

$$H_0 = \int_{-\infty}^{\infty}\left[\frac{1}{2}(\pi)^2 + \frac{1}{2}(\partial_x\varphi_0)^2 + \frac{m^2}{2}\varphi_0^2\right]\mathrm{d}x. \tag{24.12}$$

It generates the time evolution of any operator $\mathcal{O}$ via the equation of motion $\partial_t\mathcal{O} = \mathrm{i}[H_0, \mathcal{O}]$. By expanding the fields in Fourier modes and plugging back to the Hamiltonian, we recognize uncoupled harmonic oscillators. Thus we can introduce the creation and annihilation operators

$$a(k,t) = \mathrm{i}\hat{\pi}(k,t) + \omega(k)\hat{\varphi}_0(k,t), \qquad a^\dagger(k,t) = -\mathrm{i}\hat{\pi}(k,t) + \omega(k)\hat{\varphi}_0(k,t), \tag{24.13}$$

where $\omega(k) = \sqrt{k^2+m^2}$. Their non-vanishing commutation relation reads

$$[a(k,t), a^\dagger(k',t)] = (2\pi)2\omega(k)\delta(k-k'). \tag{24.14}$$

As the Hamilton takes the form

$$H_0 = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{(2\pi)2\omega(k)}\,\omega(k)\frac{1}{2}\left[a^\dagger(k,t)a(k,t) + a(k,t)a^\dagger(k,t)\right], \tag{24.15}$$

the time dependence of the creation and annihilation operators is determined exactly: $a^\dagger(k,t) = a^\dagger(k)\mathrm{e}^{\mathrm{i}\omega(k)t}$ and $a(k,t) = a(k)\mathrm{e}^{-\mathrm{i}\omega(k)t}$. The Fock Hilbert space of the model is generated from the lowest energy vacuum $|0\rangle$ as

$$a^\dagger(k_1)\cdots a^\dagger(k_n)|0\rangle = |k_1,\cdots,k_n\rangle, \qquad a(k)|0\rangle = 0. \tag{24.16}$$

Each state is an eigenstate of the energy and the momentum operators

$$\begin{aligned} H_0 &= \int_{-\infty}^{\infty} :\left[\frac{1}{2}(\partial_t\varphi_0)^2 + \frac{1}{2}(\partial_x\varphi_0)^2 + \frac{m^2}{2}\varphi_0^2\right]: \mathrm{d}x, \\ P &= \int_{-\infty}^{\infty} :\partial_x\varphi_0\partial_t\varphi_0: \mathrm{d}x \end{aligned} \tag{24.17}$$

with the eigenvalue

$$H_0|k_1,\ldots,k_n\rangle = \sum_i \omega(k_i)|k_1,\cdots,k_n\rangle, \quad P|k_1,\cdots,k_n\rangle = \sum_i k_i|k_1,\cdots,k_n\rangle. \tag{24.18}$$

Here, we normalized the energy and the momentum of the vacuum to zero. This can be achieved by introducing the normal ordering: Creation operators $a^\dagger(k)$ are put on the left of the annihilation operators $a(k')$.

The solution for the free quantum field is given by

$$\varphi_0(x,t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{(2\pi)2\omega(k)}\left[a(k)\mathrm{e}^{-\mathrm{i}\omega(k)t+\mathrm{i}kx} + a^\dagger(k)\mathrm{e}^{\mathrm{i}\omega(k)t-\mathrm{i}kx}\right]. \tag{24.19}$$

The products of operators are well-defined only if we prescribe a meaningful ordering. The time ordering is defined by

$$T\left(\varphi_0(x,t)\varphi_0(x',t')\right) = \begin{cases} \varphi_0(x,t)\varphi_0(x',t') & \text{for } t \geq t', \\ \varphi_0(x',t')\varphi_0(x,t) & \text{for } t' > t. \end{cases} \tag{24.20}$$

The free Feynman propagator (Green's function) is defined as the two-point vacuum expectation value of the time ordered product,

$$\langle 0|T\left(\varphi_0(x_1,t_1)\varphi_0(x_2,t_2)\right)|0\rangle \equiv G(t_{12},x_{12}) = \int \frac{\mathrm{d}\omega\mathrm{d}k}{(2\pi)^2}\frac{\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\omega t_{12}+\mathrm{i}kx_{12}}}{\omega^2-k^2-m^2+\mathrm{i}\epsilon}, \tag{24.21}$$

where $t_{ij} \equiv t_i - t_j$ and similarly for x. The Wick theorem allows us to calculate any correlation function as

$$\langle 0|T(\varphi_0(x_1,t_1)\cdots\varphi_0(x_{2N},t_{2N})|0\rangle = \sum_{\text{all pairings}}\left\{\prod_{\text{all } i,j \text{ pairs}} G(t_{ij},x_{ij})\right\}. \tag{24.22}$$

Thus the free model is solved completely and we are ready to define the perturbation.

24.2.2 Perturbation

The interacting theory is defined by the Lagrangian (24.9). After the Legendre transformation, we obtain the Hamiltonian[7]

$$H = H_0 + H_I = H_0 + b^2 \int \mathrm{d}x \ : U_I(\varphi) : \tag{24.23}$$

which generates time evolution. In order to have a meaningful time evolution operator (with finite matrix elements) we have to normal order the perturbing operator. This can lead to a change (renormalization) of its parameters. We also suppose that the perturbation does not change the Hilbert space of the free model and treat H_I perturbatively.

In relativistic quantum field theories, we prefer to describe the time evolution of the system in the Heisenberg picture. In this picture, the Hamiltonian generates time evolution only for operators and vectors are time independent:

$$\varphi(x,t) = \mathrm{e}^{\mathrm{i}Ht}\varphi(x,0)\mathrm{e}^{-\mathrm{i}Ht}, \qquad |k_1,\cdots,k_n;t\rangle = |k_1,\cdots,k_n;0\rangle. \tag{24.24}$$

The fact that state vectors are time independent is a manifestation of Lorentz covariance.

For technical reasons, we can switch also to the interaction picture. As the time evolution of the free system has already been solved, it can be separated from the complete Heisenberg time evolution. We evolve the operators by the free-time evolution (generated by H_0) and the vectors by the so-called evolution operator U:

$$\varphi_0(x,t) = \mathrm{e}^{\mathrm{i}H_0t}\varphi_0(x,0)\mathrm{e}^{-\mathrm{i}H_0t}, \qquad |k_1,\cdots k_n;t\rangle = U(t,0)|k_1,\ldots,k_n;0\rangle. \tag{24.25}$$

Demanding the equivalence of all matrix elements in the two descriptions we see that $U(t,0) = \mathrm{e}^{\mathrm{i}H_0t}\mathrm{e}^{-\mathrm{i}Ht}$. The time derivative of $U(t,0)$ is given by

$$\partial_t U(t,0) = -\mathrm{i}H_I(\varphi_0(t))\, U(t,0), \tag{24.26}$$

where $\varphi_0(t)$ is evolved with the free time evolution generated by H_0. As $H_I(t)$ and $H_I(t')$ do not commute in general, the solution of this differential equation can be written in terms of the time-ordered exponential:

$$U(t,0) = \mathcal{T}\exp\left\{-\mathrm{i}\int_0^t H_I\left(\varphi_0(t')\right)\mathrm{d}t'\right\}, \tag{24.27}$$

where we still have to fix the integration constant from the initial value.

The Heisenberg and interaction pictures coincide at a reference time. It is natural to choose this reference time at $-\infty$. This choice is motivated by the fact that for asymptotically large negative time particles (finite energy localized solutions traveling with different speeds) are well separated and so their interactions vanish. Taking into account the canonical normalization of the fields $[\varphi(x,t),\partial_t\varphi(x',t)] = \mathrm{i}\delta(x-x')$, we cannot suppose the complete equality, but

$$\lim_{t\to-\infty}\varphi(x,t) \approx \lim_{t\to-\infty} Z^{\frac{1}{2}}\varphi_0^{\mathrm{in}}(x,t), \tag{24.28}$$

where $0 < Z < 1$ is referred to as the wave function renormalization constant.

[7] Here we redefined U to U_I to avoid confusion with the time evolution operator.

In the perturbed theory, we are interested in the correlation functions of time ordered products of Heisenberg operators. We can again switch from the Heisenberg to the interaction picture by using the evolution operator U. As the result, we obtain

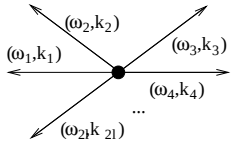
$$\begin{aligned}&\langle 0|T\left(\varphi(x_1,t_1)\cdots\varphi(x_n,t_n)\right)|0\rangle\\&\quad=\frac{\langle 0|T\left(\varphi_0(x_1,t_1)\cdots\varphi_0(x_n,t_n)\exp\left\{-\mathrm{i}\int \mathrm{d}x\,\mathrm{d}t\,\mathcal{L}_I\left(\varphi_0(x,t)\right)\right\}\right)|0\rangle}{\langle 0|T\left(\exp\left\{-\mathrm{i}\int \mathrm{d}x\mathrm{d}t\,\mathcal{L}_I\left(\varphi_0(x,t)\right)\right\}\right)|0\rangle},\end{aligned}\tag{24.29}$$

which yields a complete definition of the model. The usual way to proceed is to expand the exponential,

$$\exp\left\{-\mathrm{i}\int \mathrm{d}x\,\mathrm{d}t\,\mathcal{L}_I\left(\varphi_0(x,t)\right)\right\}=\sum_{N=0}^{\infty}\frac{(-\mathrm{i})^N}{N!}\left[\int \mathrm{d}x\,\mathrm{d}t\,\mathcal{L}_I\left(\varphi_0(x,t)\right)\right]^N\tag{24.30}$$

and to calculate any quantity perturbatively in the coupling constant. At each order, we have to calculate the vacuum expectation value of the time ordered products of free fields, which can be done with the aid of the Wick theorem (24.22). The results can be represented in terms of Feynman diagrams. For an n-point correlation function, these rules are formulated in the simplest way in the Fourier (momentum) space. They read as follows:

- Draw all topologically distinct diagrams with n outer legs
- associate the propagator $\frac{\mathrm{i}}{\omega^2-k^2-m^2+\mathrm{i}\epsilon}$ with each line



- introduce $-\mathrm{i}m^2b^{2l-2}$ for each vertex of $2l$ legs
  and demand the momentum $\sum_i k_i=0$ and energy $\sum_i\omega(k_i)=0$ conservations
- integrate over inner momenta, not fixed by momentum conservations: $\int\frac{\mathrm{d}\omega\mathrm{d}k}{(2\pi)^2}$
- divide by the symmetry factor of the graph

These rules apply only when there are no normal orderings in the Lagrangian. If we normal order the perturbation operator, we are not allowed to draw such diagrams in which a line starts and ends at the same vertex. These rules define the model perturbatively, so we can compute all correlation functions order by order.

It is instructive to compare the two types of rules and to indicate how we can regularize the theory. In the normal ordered case, one can show by simple counting that there are no divergences at all and so the theory is already well-defined. In the unrenormalized case, let us analyze the two-point propagator first. Immediately at one loop we face a divergent integral shown in Fig. 24.3:

$$\int\frac{\mathrm{d}\omega\mathrm{d}k}{(2\pi)^2}\frac{\mathrm{i}}{\omega^2-k^2-m^2+\mathrm{i}\epsilon}=\int_0^{\Lambda}\frac{\mathrm{d}k}{2\pi}\frac{1}{\sqrt{k^2+m^2}},\tag{24.31}$$

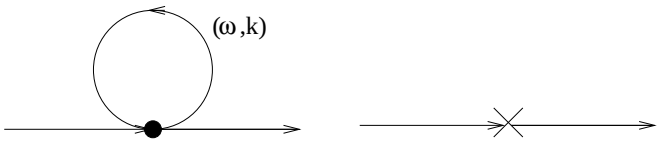


Fig. 24.3. One-loop diagram contributing to the propagator is on the left, while the diagram of its counter-term is on the right.

which was regularized by introducing a momentum cut-off Λ. But then the propagator will depend on this cut-off. To compensate this we add a Λ-dependent counter-term into the Lagrangian, namely $\delta m^2\varphi^2/2$ with

$$\delta m^2 = -m^2 b^2 \int_0^\Lambda \frac{\mathrm{d}k}{2\pi} \frac{1}{\sqrt{k^2+m^2}}. \tag{24.32}$$

Calculating other higher-point correlators at one loop we arrive at the same divergence (24.31). Interestingly, the induced counter-term in the Lagrangian for $(2n-2)$-point correlation functions is $\delta m^2 b^{2n-2}\varphi^{2n}/(2n)!$, i.e. it has exactly the same form as the original one. Thus the divergences can be absorbed into the renormalization of the mass term:

$$:V(\varphi):=: \frac{m^2}{b^2}(\cosh b\varphi - 1) := V(\varphi) - V_{\mathrm{CT}}(\varphi) = \frac{m^2-\delta m^2}{b^2}(\cosh b\varphi - 1). \tag{24.33}$$

We can calculate the renormalization of the mass order by order from the two-point propagator and use the renormalized Lagrangian to evaluate any higher-point correlation functions, which turn out to be finite. The fact that the form of the Lagrangian is not changed at the quantum level, merely the coefficients are renormalized, implies that the quantum equations of motion have the same structure as the classical ones. This shows that the sinh-Gordon theory is integrable at the quantum level, too.

The mass can be read off from the two-point function as the pole of its Fourier transform. Now we are going to derive formulas which connect the scattering matrix to the higher-point correlation functions.

24.3 Scattering matrix, reduction formulas

Classically, the particle-type excitations are well separated and non-interacting at asymptotically large times. This motivates us to adiabatically switch off the interaction for large times. We suppose that

$$\lim_{t\to\mp\infty} \varphi(x,t) \approx \lim_{t\to\mp\infty} Z^{\frac{1}{2}} \varphi_0^{\mathrm{in/out}}(x,t), \tag{24.34}$$

where Z takes care of the canonical normalization of the fields and the limit is understood in the week sense, i.e. for the matrix elements of the operators. Asymptotic annihilation/creation operators can be defined in terms of the asymptotic fields by inverting (24.13),

$$\begin{aligned} a^{\mathrm{as}}(k) &= \mathrm{i}\int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}\omega(k)t-\mathrm{i}kx} \overset{\leftrightarrow}{\partial_t} \varphi_0^{\mathrm{as}}(x,t), \\ a^{\mathrm{as}}(k)^\dagger &= -\mathrm{i}\int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}\omega(k)t+\mathrm{i}kx} \overset{\leftrightarrow}{\partial_t} \varphi_0^{\mathrm{as}}(x,t), \end{aligned} \tag{24.35}$$

where the upperscript asymptotic "as" can be either "in" ($t \to -\infty$) or "out" ($t \to +\infty$) and $f \overleftrightarrow{\partial_t} g \equiv f\partial_t g - g\partial_t f$. These operators create the asymptotic states

$$|k_1, \ldots, k_n\rangle^{\rm as} = a^{\rm as}(k_1)^\dagger \cdots a^{\rm as}(k_n)^\dagger |0\rangle. \tag{24.36}$$

In order to avoid over-counting we order the "in" basis as $k_i > k_{i+1}$ and the "out" basis oppositely $k_i < k_{i+1}$. Asymptotic completeness means that both the initial and final states form a complete set. Thus, they can be expressed in terms of each other via the scattering matrix

$$S_{\rm fi} = \langle {\rm final}|{\rm initial}\rangle. \tag{24.37}$$

As the time evolution of the states is described by the evolution operator U, the scattering matrix is nothing but

$$\begin{aligned} S = U(\infty, -\infty) &= \mathcal{T} \exp\left\{-{\rm i}\int_{-\infty}^{\infty} {\rm d}t'\, H_I\left(\varphi_0(t')\right)\right\} \\ &= \mathcal{T} \exp\left\{{\rm i}\int {\rm d}x\, {\rm d}t\, \mathcal{L}_I(\varphi_0)\right\}. \end{aligned} \tag{24.38}$$

This form implies that the S-matrix is unitary and commutes with model's symmetries.

The simplest nontrivial S-matrix element is

$${}_{\rm out}\langle k_3, k_4|k_1, k_2\rangle_{\rm in} = S(k_1, k_2|k_3, k_4)(2\pi)^2 2\omega(k_1)2\omega(k_2)\delta(k_1 - k_4)\delta(k_2 - k_3). \tag{24.39}$$

In a Lorentz invariant theory the S-matrix depends only on the relativistically invariant Mandelstam variables $s = (\omega_1 + \omega_2)^2 - (k_1 + k_2)^2$, $t = (\omega_1 - \omega_3)^2 - (k_1 - k_3)^2$ and $u = (\omega_1 - \omega_4)^2 - (k_1 - k_4)^2$, where $\omega_i \equiv \omega(k_i)$. The last two variables t and u are not independent of s in (1+1) dimensions.

The scattering matrix can be expressed in terms of the correlation functions via the so called reduction formulas, which will be derived in what follows. We first express the asymptotic creation (annihilation) operators in terms of the free asymptotic fields (24.35):

$$\begin{aligned} {}_{\rm out}\langle k_3, k_4|k_1, k_2\rangle_{\rm in} &= {}_{\rm out}\langle k_3, k_4|a^\dagger_{\rm in}(k_1)|k_2\rangle_{\rm in} \\ &= {}_{\rm out}\langle k_3, k_4|{\rm i}\int {\rm d}x\, {\rm e}^{{\rm i}\omega(k)t - {\rm i}kx} \overleftrightarrow{\partial_t}\, \varphi_0^{\rm in}(x,t)|k_2\rangle_{\rm in}, \end{aligned} \tag{24.40}$$

where k denotes the momentum we are manipulating, which in this case is k_1. The asymptotic fields can be expressed at $t = -\infty$ in terms of the interacting field (24.34). Using the identity $f(-\infty) = f(\infty) - \int_{-\infty}^{\infty} \partial_t f(t)$, the interacting field can further be expressed in terms of the disconnected, $f(\infty)$, and the connected contributions:

$$\begin{aligned} {}_{\rm out}\langle k_3, k_4|k_1, k_2\rangle_{\rm in} &= {}_{\rm out}\langle k_3, k_4|a^\dagger_{\rm out}(k_1)|k_2\rangle_{\rm in} \\ &\quad + {}_{\rm out}\langle k_3, k_4|{\rm i}Z^{-\frac{1}{2}}\int {\rm d}x\, {\rm d}t\, \partial_t \left\{{\rm e}^{{\rm i}\omega(k)t - {\rm i}kx} \overleftrightarrow{\partial_t}\, \varphi(x,t)\right\}|k_2\rangle_{\rm in}. \end{aligned} \tag{24.41}$$

In the connected piece from the second time derivative we obtain $\omega(k)^2 = k^2 + m^2$ and $\partial_t^2\varphi$. In the first term we replace k^2 by the second space derivatives, which is subsequently twice

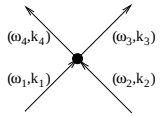


Fig. 24.4. Four-point correlation function in the leading order Feynman graph.

integrated by parts. Dropping the surface terms (as the fields are vanishing at infinities) we obtain

$$ {}_{\rm out}\langle k_3,k_4|k_1,k_2\rangle_{\rm in} = \text{disconnected} + {\rm i}Z^{-\frac{1}{2}}\mathcal{D}_{\rm out}\langle k_3,k_4|\varphi(x,t)|k_2\rangle_{\rm in}, \tag{24.42} $$

where

$$ \mathcal{D} = -\int {\rm d}x\,{\rm d}t\,{\rm e}^{-{\rm i}\omega(k)t+{\rm i}kx}\Box, \qquad -\Box = -\partial_t^2+\partial_x^2-m^2. \tag{24.43} $$

Repeating the same procedure for each asymptotic creation/annihilation operator we obtain the final form of the reduction formula

$$ \begin{aligned} {}_{\rm out}\langle k_3,k_4|k_1,k_2\rangle_{\rm in} &= (2\pi)^2 2\omega(k_1)2\omega(k_2)\delta(k_1-k_4)\delta(k_2-k_3) \\ &\quad + Z^{-2}\bar{\mathcal{D}}_4\bar{\mathcal{D}}_3\mathcal{D}_2\mathcal{D}_1\langle 0|T\left(\varphi(1)\varphi(2)\varphi(3)\varphi(4)\right)|0\rangle, \end{aligned} \tag{24.44} $$

where $\varphi(i)$ stands for $\varphi(x_i,t_i)$, $\mathcal{D}_i=\mathcal{D}(x\to x_i)$ and similarly for $\Box_i$. The physical meaning of the operator $\mathcal{D}_i$ is to truncate the correlation function and to put them on-shell. Clearly, in the momentum space $\Box_i$ picks up the residue of the pole of the propagator, while the inverse Fourier transformation puts the particle on the mass shell: $\omega^2+k^2=m^2$. For initial states we obtain the operator $\bar{\mathcal{D}}_i=-\int {\rm d}x_i\,{\rm d}t_i\,{\rm e}^{{\rm i}\omega(k_i)t_i-{\rm i}k_ix_i}\Box_i$. The only difference between the operators $\mathcal{D}_i$ and $\bar{\mathcal{D}}_i$ consists in the sign of the energy-momentum vector (ω,k). From this fact we can read off the crossing symmetry of the scattering matrix,

$$ S(k_1,k_2|k_3,k_4) = S(k_1,\bar{k}_3|\bar{k}_2,k_4), \tag{24.45} $$

where the energy-momentum vector of the anti-particle is $\bar{k}\to(-\omega(k),-k)$.

We have already developed the technique to calculate the correlation functions. Using the reduction formula, we can elaborate order by order the scattering matrix of the sinh-Gordon theory. Let us calculate the four-point correlation function at the leading order. The contribution of the Feynman graph in Fig. 24.4 to the momentum space 4-point function is

$$ \begin{aligned} G^4(\{\omega_i\},\{k_i\}) &= (-{\rm i}m^2b^2)(2\pi)^2\delta(\omega_1+\omega_2-\omega_3-\omega_4)\delta(k_1+k_2-k_3-k_4) \\ &\quad \times\prod_{i=1}^4\frac{i}{\omega_i^2-k_i^2-m^2+{\rm i}\epsilon}. \end{aligned} \tag{24.46} $$

The reduction formula multiplies each leg by the factor $\omega_i^2-k_i^2-m^2$ and puts all momenta on the mass shell $\omega_i^2-k_i^2\to m^2$. As the result, the amplitude is proportional to the product of delta functions with $\omega\to\omega(k)$. Notice, however, that in the definition of the S-matrix (24.39) we have different delta functions. The relation is simply

$$ \begin{aligned} &\delta\left(\omega(k_1)+\omega(k_2)-\omega(k_3)-\omega(k_4)\right)\delta(k_1+k_2-k_3-k_4) \\ &\qquad = \frac{1}{\omega'(k_1)-\omega'(k_2)}\delta(k_1-k_3)\delta(k_2-k_4). \end{aligned} \tag{24.47} $$

Thus the scattering matrix in the leading order in b is

$$S(k_1,k_2|k_3,k_4) = 1 - \mathrm{i}\frac{b^2}{4}\frac{1}{\sinh(\theta_1-\theta_2)}, \tag{24.48}$$

where the unity is obtained from the disconnected part and the rapidity parameterization $k = m\sinh\theta$ was used. We can calculate systematically also higher-order corrections [32, 33].

24.4 The analytic structure of the scattering matrix

In the previous section, we introduced the Feynman perturbation rules for calculating the correlation functions, which then can be used to calculate the scattering matrix via the reduction formula. Now, following [45], we analyze what sort of singularities can exhibit various terms in the perturbative expansion and how they are summed up to the singularity of correlation functions and the scattering matrix.

Let us analyze a Feynman diagram of N outer on-shell legs with momenta $k_1,\dots,k_N$. The leg-truncated amplitude can be calculated in the perturbation theory as

$$A = \prod_{i=1}^{L}\int \frac{\mathrm{d}\nu_i\,\mathrm{d}q_i}{(2\pi)^2}\prod_{j=1}^{J}(\omega_j^2 - p_j^2 - m^2 + \mathrm{i}\epsilon)^{-1}, \tag{24.49}$$

where (ν_i, q_i) denotes one of L loop momenta, while (ω_j, p_j) denotes the energy and momentum of one of J inner lines. As the theory is relativistically invariant the amplitude depends only on the combinations $\omega(k_i)\omega(k_j) - k_ik_j$. This property can be made explicit by introducing the Feynman parameterization

$$A = \prod_{i=1}^{L}\int \frac{\mathrm{d}\nu_i\mathrm{d}q_i}{(2\pi)^2}\prod_{j=1}^{J}\int_0^1 \mathrm{d}\alpha_j\,\delta\left(\sum\alpha_j - 1\right)\left[\sum_{j=1}^{J}\alpha_j(\omega_j^2 - p_j^2 - m_j^2 + \mathrm{i}\epsilon)\right]^{-J} \tag{24.50}$$

and by evaluating the (ν_i, q_i) loop integrals. The UV divergences can be regularized by the already introduced counter-terms or by normal ordering the perturbation operator. Thus the expression is finite provided $\epsilon > 0$. In the physical $\epsilon \to 0$ limit, however, singularities of the integrand can cross the α hyper-contour. These singularities can be avoided by continuously deforming the contour provided that the contour is not pinched or the singularity is not localized at the boundary of integration. Thus physical singularities appear whenever

$$\alpha_j = 0 \qquad \text{or} \qquad \omega_j^2 - p_j^2 - m^2 = 0 \quad \text{and} \quad \partial_i\sum_{j=1}^{J}\alpha_j(\omega_j^2 - p_j^2 - m_j^2) = 0, \tag{24.51}$$

where ∂_i is both ∂_{ν_i} and ∂_{q_i}. These are the so-called Landau equations which formulate the singularities of the Feynman diagrams. They have a clear physical meaning. To understand them we shrink every line with $\alpha_j = 0$ to a point. The resulting graph is called the reduced graph. Graphs which are transformed to the same reduced graph have the same singularity structure. The shrunk lines sum up to the exact vertex functions. Clearly in a reduced graph all particles are on shell.

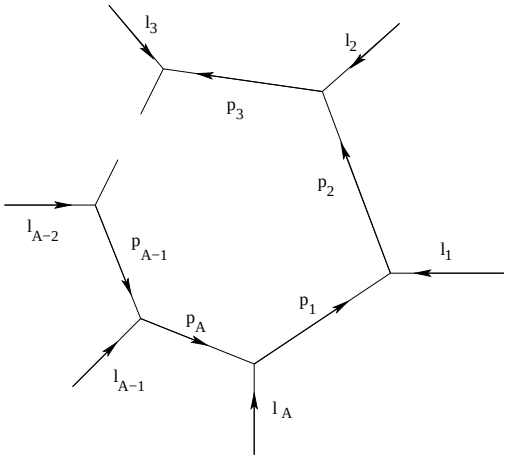


Fig. 24.5. Generic closed loop. Lines are labeled by momenta.

Let us consider a generic loop l_i in a reduced graph, see Fig. 24.5. We use the momentum conservation at each vertex to express all inner momenta in terms of p_1 as

$$p_2 = p_1 + l_1, \quad p_3 = p_2 + l_2 = p_1 + l_1 + l_2, \cdots \quad p_A = p_1 + \sum_{j=1}^{A-1} l_j. \tag{24.52}$$

The total momentum is evidently conserved: $\sum_i l_i = 0$. The Landau equation for $q_i = p_1$ reads as

$$\sum_{\text{each loop}} \alpha_i p_i = 0; \tag{24.53}$$

we have similar equations for the energy components, too. Coleman and Norton [46] have a nice interpretation of these equations: The physical singularities of the correlation functions ($\alpha_i \geq 0$) correspond to such space-time diagrams in which all particles propagate on shell, forward in time, and interact with each other in space-time points via energy and momentum conserving interactions. To visualize such a picture we draw for each inner line a vector $(\alpha_i \omega_i, \alpha_i p_i)$ of length $\alpha_i m$. Lines with $\alpha = 0$ are shrunk to a point. A space-time interaction point is associated with each vertex in the graph. The Landau equation guaranties that they are well defined, as different paths define the same point.

The Cutkosky rules describe the discontinuity caused by such graphs. One has to calculate the singularity of the graph as if it were a Feynman diagram but with replacing the interaction vertices by exact (all graphs summed up) vertices and the propagator by $2\pi\theta(\omega)\delta(\omega^2 - p^2 - m^2)$.

Boundstates show up as singularities in the two-particle scattering matrix with purely imaginary relative rapidities. They also can be interpreted as Landau singularities. In this case, if say $\theta_1 = -\mathrm{i}u_1$ and $\theta_2 = \mathrm{i}u_2$, the momenta are purely imaginary $p_1 = \mathrm{i}q_1 = \mathrm{i}m \sin u_1$ and the energy - momentum vector (ω_1, q_1) can be drawn in the two-dimensional Euclidean space, where it has the length m. Diagrams explaining the singularities of the scattering matrix in this

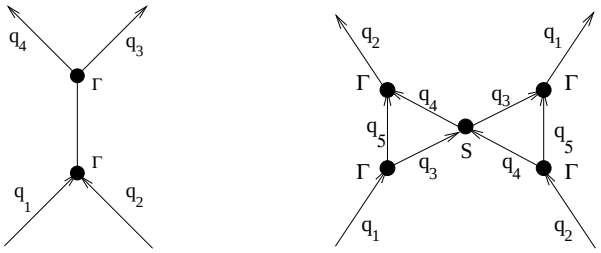


Fig. 24.6. Boundstate diagram on the left, a more complicated Coleman-Thun diagram on the right.

kinematics are called Coleman-Thun diagrams [47]. A boundstate diagram is shown on the left of Fig. 24.6. Let us suppose that the pole of the scattering matrix appears at $\mathrm{i}u$, that is $u_1 = \frac{u}{2}$ and $u_2 = -\frac{u}{2}$. Since at the space-time points the energy and momentum are conserved, the momentum of the boundstate is zero and the energy is nothing but its mass

$$m_{\mathrm{bs}} = 2m \cos \frac{u}{2}. \tag{24.54}$$

The boundstate has the same mass as the original particle if $u = \pi/3$. We can also check the singularity of the boundstate diagram according to the Cutkosky rules. As we have just one line in the graph we obtain one delta function, which is the discontinuity of a single pole singularity:

$$S(\theta)\big|_{\theta=\mathrm{i}\pi/3} = \mathrm{i}\frac{\Gamma^2}{\theta - \mathrm{i}\pi/3} + \cdots, \tag{24.55}$$

where Γ is the exact three-point vertex.

There are other more complicated Coleman-Thun diagrams, like the one shown on the right of Fig. 24.6. The divergence in this case is a second-order pole as we have six propagators and two loop integrals for the energy and momentum. The strength of the pole is proportional to $\Gamma^4 S(q_3, q_4)$.

25 Bootstrap quantization

Let us summarize what we learnt from the previous section devoted to the quantum sinh-Gordon theory. The Hilbert space of the theory can be identified with non-interacting multiparticle states. All scattering states for asymptotically large negative and positive times consist of well-separated localized particles which do not interact. The initial and final multiparticle states are connected by the scattering S-matrix, whose semiclassical limit is related to the time shift. The scattering matrix is unitary and satisfies crossing symmetry. As S corresponds to the amputed on-shell correlation function, it is singular only when a Coleman-Thun type diagram can be drawn with the given kinematics. Since the potential of the renormalized quantum sinh(sine)-Gordon theory has the same form as the classical one, we expect that is integrable. Integrability is also supported by the analysis of Sect. 23, where we have shown the existence of higher-spin conserved charges. Our next aim is to analyze additional requirements coming from the existence of an infinite family of conserved charges and to build up an axiomatic framework [31,48,49] which eventually leads to the complete solution for the sine-Gordon S-matrix.

25.1 Asymptotic states, scattering matrix

First we set up a general background. The Hilbert space of the model is spanned by free multiparticle states. For simplicity, we start with just one single relativistic particle of mass m. (This is what we expect in the quantum sinh-Gordon theory). The model is relativistically invariant, thus the dispersion relation can be written as

$$E(p) = \omega(p) = \sqrt{p^2 + m^2}, \qquad E(p)^2 - p^2 = m^2. \tag{25.1}$$

Using the rapidity parameterization, we have

$$E(\theta) = \omega(\theta) = m\cosh\theta, \qquad p(\theta) = m\sinh(\theta). \tag{25.2}$$

Light-cone components diagonalize the action of boosts and can be written as

$$(E \pm p)(\theta) = Q_{\pm 1}(\theta) = m\mathrm{e}^{\pm\theta}. \tag{25.3}$$

In an integrable theory these are the first members of an infinite family of conserved charges which can be labeled by their spin s: $Q_s(\theta) = q_s\mathrm{e}^{s\theta}$.

We suppose the asymptotic completeness, i.e. the asymptotic initial and final multiparticle states span the Hilbert space. Introducing their abstract creation operators, an initial state, in which the particles are ordered according to their rapidities, can be written as

$$A^\dagger_{\mathrm{in}}(\theta_1)\cdots A^\dagger_{\mathrm{in}}(\theta_n)|0\rangle = |\theta_1,\cdots,\theta_n\rangle_{\mathrm{in}}, \qquad \theta_1 > \cdots > \theta_n, \tag{25.4}$$

where the fastest particle is on the left. In the final state

$$A^\dagger_{\mathrm{out}}(\theta_1)\cdots A^\dagger_{\mathrm{out}}(\theta_m)|0\rangle = |\theta_1,\cdots,\theta_m\rangle_{\mathrm{out}}, \qquad \theta_m > \cdots > \theta_1, \tag{25.5}$$

after all scatterings have been performed, the particles are ordered oppositely, i.e. the fastest one is on the right. Both bases diagonalize the action of the infinite family of conserved charges, e.g.

$$Q_s|\theta_1,\cdots,\theta_n\rangle_{\mathrm{in}} = \sum_{i=1}^{n} q_s\mathrm{e}^{s\theta_i}|\theta_1,\cdots,\theta_n\rangle_{\mathrm{in}}. \tag{25.6}$$

The scattering matrix connects the two bases of the Hilbert space, simply it relates the initial and final states:

$$S_{n\to m} = {}_{\rm out}\langle\theta'_1,\cdots,\theta'_m|\theta_1,\cdots,\theta_n\rangle_{\rm in}. \tag{25.7}$$

Its absolute square describes the probability with which the initial state evolves into the final state.

25.2 S-matrix properties

Here we list all necessary requirements the S-matrix has to satisfy and their consequences.

25.2.1 Basic symmetries

As the scattering matrix is the time evolution operator in the interaction picture, it is built up from the interacting Hamiltonian. A direct consequence is its symmetry: S must commute with the generators of symmetries, namely the conserved charges Q_s. Thus if we evaluate the charges before and after the scattering, they have to coincide:

$$\sum_{i=1}^{n} q_s \mathrm{e}^{s\theta_i} = \sum_{j=1}^{m} q_s \mathrm{e}^{s\theta'_j}. \tag{25.8}$$

These are functionally independent polynomial equations ($x_i = \mathrm{e}^{\theta_i}$) for an infinite number of different values of the spin s. They can be satisfied for a finite number of $\{\theta_i\}$ and $\{\theta'_j\}$ only if the two sets are completely equivalent: $\{\theta_i\} = \{\theta'_j\}$. In particular, the number of particles in the initial and final states coincides, $n = m$, i.e. there is no particle creation in integrable quantum theories.

Conserved charges generate symmetry transformations. For $s = \pm 1$, H generates a uniform shift in time while P generates a uniform shift in space. Higher-spin charges, however, generate momentum dependent shifts in space-time [49]. Because all rapidities are different, by acting with a higher-spin charge we can spatially separate the particle interactions and factorize the multiparticle scattering amplitudes into the product of two particle scatterings:

$$S_{n\to n}(\theta_1,\cdots,\theta_n) = \prod_{\text{all (i,j) pairs}} S_{2\to 2}(\theta_i,\theta_j). \tag{25.9}$$

The full information about the multiparticle scattering is thus contained in the two-particle elastic scattering matrix $S_{2\to 2}(\theta_1,\theta_2)$ to which we shall restrict ourselves from now on. The Lorentz invariance acts on the rapidity as $\theta \to \theta + \Lambda$ and, as it is a model symmetry, we can write

$$S_{2\to 2}(\theta_1,\theta_2) = S(\theta_1 - \theta_2). \tag{25.10}$$

In a perturbative calculation the scattering matrix will depend on the Mandelstam variable

$$s = (E_1 + E_2)^2 - (p_1 + p_2)^2 = 2m^2(1 + \cosh\theta), \qquad \theta = \theta_1 - \theta_2. \tag{25.11}$$

Calculating perturbatively the scattering matrix, the s-dependence comes from propagators of the form $(\omega^2 - k^2 + s - m^2 + \mathrm{i}\epsilon)^{-1}$. The perturbation theory also shows that the scattering matrix has a cut just on the real axis, starting from $s = 4m^2$ and its physical value can be taken just above the cut when $\epsilon \to 0^+$.

25.2.2 Unitarity

If we take the physical value of S just below the cut (like in the $-\mathrm{i}\epsilon$ description), we would obtain the time reversed process (anti-time ordering), which, by unitarity, must be the inverse of the original process. Thus extending the definition of the scattering matrices to complex θ arguments, the requirement of unitarity reads as

$$S(\theta)S(-\theta) = 1. \tag{25.12}$$

This relation is due to the fact that the two sides of the cut are mapped to θ and $-\theta$, respectively.

25.2.3 Crossing symmetry

We can analyze the crossed version of the scattering process in which the Mandelstam variable s is replaced by $t = 4m^2 - s$. In the language of the generalized rapidity, it amounts to the change $\theta \to \mathrm{i}\pi - \theta$. Thus the crossing symmetry reads as

$$S(\theta) = S(\mathrm{i}\pi - \theta). \tag{25.13}$$

The symmetry can be deduced also from the particle $\leftrightarrow$ anti-particle transformation which, in the language of the rapidity, reads as $(\omega(\theta), p(\theta)) \to (-\omega(\theta), p(\theta)) = (\omega(\mathrm{i}\pi - \theta), p(\mathrm{i}\pi - \theta))$.

25.2.4 Maximal analyticity

The scattering matrix $S(\theta)$ is a meromorphic function of the rapidity variable on the physical strip $0 < \Im m(\theta) < \pi$, having poles on the imaginary axis only. Each pole must correspond to Coleman-Thun diagrams and can be either a boundstate or an anomalous threshold. The physical value of the scattering matrix is given by $\lim_{\epsilon\to 0} S(\theta + \mathrm{i}\epsilon)$ for $\Re e(\theta) > 0$ and for the crossed process by $\lim_{\epsilon\to 0} S(\theta + \mathrm{i}(\pi - \epsilon)$ for $\Re e(\theta) < 0$.

25.2.5 Yang-Baxter equation

In general, when we have not just one type of particles (like the soliton and anti-soliton in the sine-Gordon theory), the factorization of the scattering matrix provides severe restrictions. These are the YB equations. As usual, they reflect that the $3 \to 3$ particle scattering can be factorized in two inequivalent ways:

$$S_{12}(\theta_{12})S_{13}(\theta_{13})S_{23}(\theta_{23}) = S_{23}(\theta_{23})S_{13}(\theta_{13})S_{12}(\theta_{12}), \tag{25.14}$$

which can be read off from Fig. 25.1.

25.3 Solving the simplest models by bootstrap

Now we try to find the scattering matrices which satisfy all above requirements.

The simplest solution is just

$$S(\theta) = 1. \tag{25.15}$$

This scattering matrix corresponds to a meaningful theory, namely to the free boson (the Klein-Gordon theory).

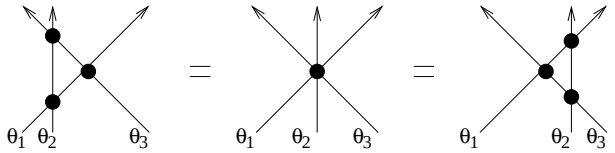


Fig. 25.1. The factorization of the $3 \to 3$ particle scattering process.

As the next simplest case, we look for the solution of the form $S(\theta) = f(\theta)/f(-\theta)$, which automatically satisfies unitarity. To fulfil the crossing relation, we introduce the variable $x = \mathrm{e}^{\theta}$ and demand $f(x)$ to be invariant under the transformation $x \to -x^{-1}$. The simplest function possessing this property is $f(x) = a + x - x^{-1}$ which includes a free parameter a. In the rapidity variable, the solution reads as

$$S(\theta) = \frac{\sinh\theta - \mathrm{i}\sin\alpha}{\sinh\theta + \mathrm{i}\sin\alpha}, \qquad \alpha > 0. \tag{25.16}$$

The choice of real $\alpha > 0$ ensures no singularity in the physical strip. The corresponding QFT is a quantum integrable model with particles of one type only. We claim that the scattering matrix corresponds to the sinh-Gordon theory if

$$\alpha = \frac{\pi b^2}{8\pi + b^2}. \tag{25.17}$$

We can check this result at the leading order in b using the result (24.48) of the previous section. The perturbative analysis was extended up to 3 loops [50], a complete check can be obtained only through the sine-Gordon theory. In order to analyze the sine-Gordon theory we analytically continue in the coupling $b \to \mathrm{i}b$.

The only particle of the sinh-Gordon theory corresponds to the fundamental field excitation of the sine-Gordon theory, which is the quantum analogue of the breather; we shall denote this "first" breather by B_1. After the analytical continuation in b, the relation between the parameters of the Lagrangian and the scattering matrix takes the form $\alpha = -(\pi b^2)/(8\pi - b^2)$. Since $\alpha < 0$ we have a pole in the physical strip on the imaginary axis at $\theta = -\mathrm{i}\alpha$. We interpret this pole as a boundstate and associate to it a new particle in the spectrum; let us call it the second breather B_2. It is an asymptotic state which must be included into the Hilbert space of the theory. A standing B_2 is composed of two B_1's with rapidities $\mathrm{i}\alpha/2$ and $-\mathrm{i}\alpha/2$, thus its mass is simply

$$m_{B_2} = 2m_{B_1}\cos\frac{\alpha}{2}. \tag{25.18}$$

A moving B_2 particle with rapidity θ is composed of one B_1 with rapidity $\theta + \mathrm{i}\alpha/2$ and another one with rapidity $\theta - \mathrm{i}\alpha/2$, which can be deduced from its momentum $m_{B_2}\sinh\theta$. As the conserved charges sum up, the generic spin s charge has its eigenvalue $2q_s\mathrm{e}^{s\theta}\cos(s\alpha/2)$ for the B_2 particle with rapidity θ.

The scattering matrix of B_2 can be calculated by the bootstrap principle. Since higher-spin conserved charges shift the trajectories in a momentum-dependent way without altering the scattering process, we can calculate the B_2B_1 scattering as shown in Fig. 25.2. As a result, we obtain

$$S_{B_2B_1}(\theta' - \theta) = S_{B_1B_1}\left(\theta' - \theta + \mathrm{i}\frac{\alpha}{2}\right) S_{B_1B_1}\left(\theta' - \theta - \mathrm{i}\frac{\alpha}{2}\right). \tag{25.19}$$

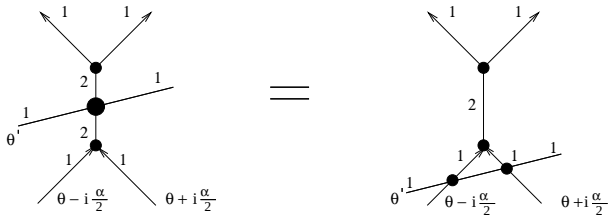


Fig. 25.2. Bootstrap method to calculate the scattering matrix of the boundstate from the scattering matrices of its constituents.

Similar calculation yields

$$S_{B_2B_2}(\theta'-\theta) = S_{B_2B_1}\left(\theta'-\theta+\mathrm{i}\frac{\alpha}{2}\right) S_{B_2B_1}\left(\theta'-\theta-\mathrm{i}\frac{\alpha}{2}\right). \tag{25.20}$$

One can ask the question whether B_2 is really a new particle? Indeed, if $S_{B_1B_2} = S_{B_1B_1}$ there is no need to introduce B_2, it can be simply identified with B_1. Actually this happens for the coupling $\alpha = -2\pi/3$. This theory, the scaling Lee-Yang model [34, 51], is consistent: All poles of the scattering matrix corresponds to boundstates.

If $\alpha \neq -\frac{2\pi}{3}$, we have to consider the second breather B_2 as a new particle and include it into the spectrum of the theory. Then we analyze the pole structure of $S_{B_1B_2}$ and $S_{B_2B_2}$: To each pole we have to associate either a boundstate or an anomalous threshold (the Coleman-Thun diagram). Once we managed to find all particles of the spectrum by using this procedure, in such a way that all singularities in all scattering matrices are explained, the theory is solved. The procedure is called the S-matrix bootstrap.

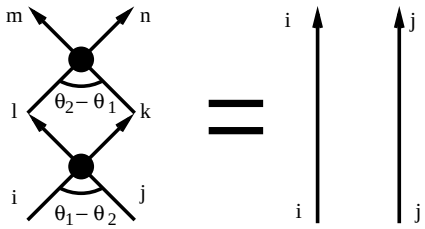
In the particular case of irrational α, we cannot close the bootstrap program purely on the boundstates having their origin in the first breather B_1. Thus the theory with S-matrix (25.16) is not consistent if we do not include the soliton and the anti-soliton. In the next subsection, we start with the soliton and anti-soliton particles and compute their scattering matrix respecting its consistencies.

25.4 The sine-Gordon *S*-matrix

Now we want to push forward the boostrap procedure for the sine-Gordon theory. We learnt from the classical theory that there are in the spectrum two particles with the same mass, namely the soliton and the anti-soliton. They carry different topological charges and in the quantum theory they will form a doublet A_i $(i = \pm)$. Their scattering can be encoded into the scattering matrix

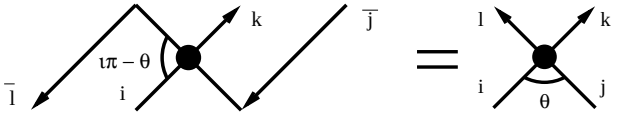
$$S_{ij}^{kl}(\theta_1-\theta_2) \qquad \begin{matrix} \mathrm{l} & & \mathrm{k} \\ & \theta_1-\theta_2 & \\ \mathrm{i} & & \mathrm{j} \end{matrix},$$

which is a four by four matrix. The unitarity equation takes the form:



$$S_{ij}^{kl}(\theta_1-\theta_2)S_{lk}^{nm}(\theta_2-\theta_1)=\delta_i^m\delta_j^n. \tag{25.21}$$

In the case of the crossing symmetry we have to take into account that, as the names suggest, the soliton is the anti-particle of the anti-soliton:



$$S_{\bar{l}i}^{\bar{j}k}(\mathrm{i}\pi-\theta)=S_{ij}^{kl}(\theta), \tag{25.22}$$

where the antiparticle of $l=\pm$ is denoted by $\bar{l}=\mp$.

Now we use model's symmetries to restrict the possible forms of the scattering matrix. We suppose that the topological charge $Q_{\rm top}|\pm\rangle=\pm|\pm\rangle$ is conserved. This means that evaluating the charge before and after the scattering we obtain the same result. In particular, for the scattering $S_{ij}^{kl}(\theta)$ we must have $i+j=k+l$. Similarly, the parity and the charge conjugation are also important symmetries. This means that the soliton and anti-soliton must scatter with the same amplitude. The most general scattering matrix possessing these properties has the form

$$\begin{aligned} S(\theta) &= \begin{pmatrix} S_{++}^{++}(\theta) & 0 & 0 & 0 \\ 0 & S_{+-}^{+-}(\theta) & S_{+-}^{-+}(\theta) & 0 \\ 0 & S_{-+}^{+-}(\theta) & S_{-+}^{-+}(\theta) & 0 \\ 0 & 0 & 0 & S_{--}^{--}(\theta) \end{pmatrix} \\ &= \rho(\theta)\begin{pmatrix} a(\theta) & 0 & 0 & 0 \\ 0 & b(\theta) & c(\theta) & 0 \\ 0 & c(\theta) & b(\theta) & 0 \\ 0 & 0 & 0 & a(\theta) \end{pmatrix}. \end{aligned} \tag{25.23}$$

Additional restrictions to the scattering matrix have their origin in the Yang-Baxter equation

$$S_{ij}^{pr}(\theta_1-\theta_2)S_{pk}^{lq}(\theta_1-\theta_3)S_{rq}^{mn}(\theta_2-\theta_3)=S_{jk}^{pr}(\theta_2-\theta_3)S_{ir}^{qn}(\theta_1-\theta_3)S_{qp}^{lm}(\theta_1-\theta_2), \tag{25.24}$$

together with unitarity

$$\begin{aligned} S_{++}^{++}(\theta)S_{++}^{++}(-\theta) &= 1, \\ S_{+-}^{+-}(\theta)S_{+-}^{+-}(-\theta)+S_{+-}^{-+}(\theta)S_{-+}^{+-}(-\theta) &= 1, \\ S_{+-}^{+-}(\theta)S_{-+}^{+-}(-\theta)+S_{+-}^{-+}(\theta)S_{+-}^{+-}(-\theta) &= 0 \end{aligned} \tag{25.25}$$

and crossing symmetry

$$S_{++}^{++}(\mathrm{i}\pi-\theta)=S_{+-}^{+-}(\theta),\qquad S_{+-}^{-+}(\mathrm{i}\pi-\theta)=S_{-+}^{+-}(\theta). \tag{25.26}$$

The YBE is an overdetermined system of equations, which in this particular case has three types of solutions: The rational, the trigonometric and the elliptic ones. To cover the sine-Gordon theory, we need the trigonometric solution:

$$a(\theta)=1,\qquad b(\theta)=-\frac{\sin(\mathrm{i}\lambda\theta)}{\sin\lambda(\pi+\mathrm{i}\theta)},\qquad c(\theta)=\frac{\sin(\lambda\pi)}{\sin\lambda(\pi+\mathrm{i}\theta)}. \tag{25.27}$$

Here, λ is a parameter which will be related to the b parameter of the sine-Gordon Lagrangian. The scalar prefactor $\rho(\theta)$ is fixed by the unitary and crossing conditions:

$$\rho(\theta)\rho(-\theta)=1,\qquad \rho(\mathrm{i}\pi-\theta)=-\rho(\theta)\frac{\sin(\mathrm{i}\lambda\theta)}{\sin\lambda(\pi+\mathrm{i}\theta)}. \tag{25.28}$$

We are interested in the solution in the physical strip $\Im m(\theta)<\pi$. Combining the two equations we can write

$$\rho\left(\theta+\frac{i\pi}{2}\right)\rho\left(\theta-i\frac{\pi}{2}\right)=-\frac{\sin(\mathrm{i}\lambda\theta+\lambda\pi/2)}{\sin(\mathrm{i}\lambda\theta-\lambda\pi/2)}. \tag{25.29}$$

First we suppose that $\lambda<1$ in order to avoid poles and zeros of the rhs in the strip $\Im m(\theta)<\pi/2$. We also suppose that ρ is non-zero and analytical in this strip as we are looking for the minimal solution of our equations. We take the logarithm of both sides

$$\ln\left(\rho\left(\theta+\frac{\mathrm{i}\pi}{2}\right)\right)+\ln\left(\rho\left(\theta-\frac{\mathrm{i}\pi}{2}\right)\right)=\ln\left[-\frac{\sin(\mathrm{i}\lambda\theta+\lambda\pi/2)}{\sin(\mathrm{i}\lambda\theta-\lambda\pi/2)}\right]. \tag{25.30}$$

The shift operator $Df(\theta)=f(\theta+\mathrm{i}\pi/2)+f(\theta-\mathrm{i}\pi/2)$ can be inverted in the Fourier space provided that the function $\ln\rho(\theta)$ has a good asymptotic at infinity. Using also that

$$\ln\left(\frac{\sin[(\pi x-\mathrm{i}\theta)/2]}{\sin[(\pi x+\mathrm{i}\theta)/2]}\right)=\int_0^\infty\frac{\mathrm{d}t}{t}\frac{\sinh t(1-x)}{\sinh t}\sinh\left(\frac{t\theta}{\mathrm{i}\pi}\right), \tag{25.31}$$

we obtain the minimal solution for ρ:

$$\rho(\theta)=-\exp\left\{\int_0^\infty\frac{\mathrm{d}t}{t}\frac{\sinh t(1+\lambda)}{\sinh t\,\cosh t\lambda}\sinh\left(\frac{2\lambda t\theta}{\mathrm{i}\pi}\right)\right\}, \tag{25.32}$$

where the sign cannot be fixed from this analysis. We can multiply the solution by every function which satisfies $f(\theta)f(-\theta)=1$ and $f(\mathrm{i}\pi-\theta)=f(\theta)$. This non-uniqueness is known as the CDD ambiguity. We take the simplest possible solution and check the consequences.

If we keep the parameter λ in the range $\lambda<1$, the S-matrix has no singularity in the physical strip and the theory is completely solved. In particular, this is true for $S_{+-}^{-+}(\theta)$ which shows that in the considered parameter range the soliton and the antisoliton cannot form any boundstate. This is the repulsive regime of the sine-Gordon theory.

The domain $\lambda>1$ is called the attractive regime of the sine-Gordon theory.

If λ lies in the range $1<\lambda<2$, the soliton–anti-soliton scatterings $S_{+-}^{+-}(\theta)=\rho(\theta)b(\theta)$ and $S_{+-}^{-+}(\theta)=\rho(\theta)c(\theta)$ have one pole at $\theta=\mathrm{i}\pi(1-\lambda^{-1})$. We associate a bound-state to this pole,

which is the quantum analogue of the breather. Using the bootstrap principle we can calculate the mass of the boundstate in terms of the soliton (anti-soliton) mass M as follows

$$m_{B_1} = 2M\cos\left(\frac{\pi}{2} - \frac{\pi}{2\lambda}\right) = 2M\sin\left(\frac{\pi}{2\lambda}\right). \tag{25.33}$$

The bootstrap also tells us how to calculate the soliton-breather scattering matrix:

$$S_{+1}^{+1}(\theta) = S_{++}^{++}\left(\theta - \mathrm{i}\frac{\pi}{2}\left(1 - \frac{1}{\lambda}\right)\right) S_{+-}^{+-}\left(\theta + \mathrm{i}\frac{\pi}{2}\left(1 - \frac{1}{\lambda}\right)\right) = S_{-1}^{-1}(\theta). \tag{25.34}$$

Interestingly, the formula simplifies itself considerably:

$$S_{+1}^{+1}(\theta) = -\frac{\sin\left(\frac{\pi}{4}\left(1+\frac{1}{\lambda}\right) - \mathrm{i}\frac{\theta}{2}\right)\sin\left(\frac{\pi}{4}\left(1-\frac{1}{\lambda}\right) - \mathrm{i}\frac{\theta}{2}\right)}{\sin\left(\frac{\pi}{4}\left(1+\frac{1}{\lambda}\right) + \mathrm{i}\frac{\theta}{2}\right)\sin\left(\frac{\pi}{4}\left(1-\frac{1}{\lambda}\right) + \mathrm{i}\frac{\theta}{2}\right)}. \tag{25.35}$$

Inspecting the analytical structure of the above scattering, the appearing poles do not signal more boundstates in the range $1 < \lambda < 2$. One can calculate also the B_1B_1 scattering from the bootstrap, with the result

$$S_{11}^{11}(\theta) = \frac{\sinh\theta + \mathrm{i}\sin(\pi/\lambda)}{\sinh\theta - \mathrm{i}\sin(\pi/\lambda)}. \tag{25.36}$$

This is indeed the analytical continuation of the expected sinh-Gordon scattering matrix (25.16). We anticipate λ to be related to the Lagrangian parameter b as

$$\lambda = \frac{8\pi}{b^2} - 1, \tag{25.37}$$

which will be derived in the next section. As has been already discussed, the scattering matrix $S_{11}^{11}(\theta)$ has a pole at $\theta = \mathrm{i}\pi/\lambda$ which lies in the physical strip. We cannot associate to this pole another particle of breather type since such a particle should have shown up already in the soliton–anti-soliton scattering (where we found the first breather only). Thus we have to find the corresponding Coleman-Thun diagram to explain the singularity. The diagram pictured on the right of Fig. 24.6 is a candidate. Actually, there exist two diagrams in which the soliton and anti-soliton propagate in the triangle. Individually, each diagram would give a second-order pole, but the sum of the S-matrices in the middle of the figure has a zero, which renders the singularity to the first order, as expected [49]. In this way we explained all singularities of all scattering matrices. The bootstrap program is closed and we solved the sine-Gordon theory in the interval $1 < \lambda < 2$. The spectrum in this range contains the soliton, the anti-soliton and a breather.

When increasing λ further, the soliton–anti-soliton scatterings have poles at $\theta = \mathrm{i}\pi[1 - (n/\lambda)]$. For a given λ, these poles are in the physical strip if $n = 1, \ldots, [\lambda]$[8]. This signals the presence of $[\lambda]$ breather boundstates $B_1, B_2, \cdots, B_{[\lambda]}$. These boundstates are the quantized counterparts of the classical breather labelled by the continuous parameter v. The masses of these boundstates can be calculated from the fusion angle,

$$m_{B_n} = 2M\sin(u_n), \qquad u_n = \frac{n\pi}{2\lambda}. \tag{25.38}$$

[8]Here $[\lambda]$ denotes the integer part of λ.

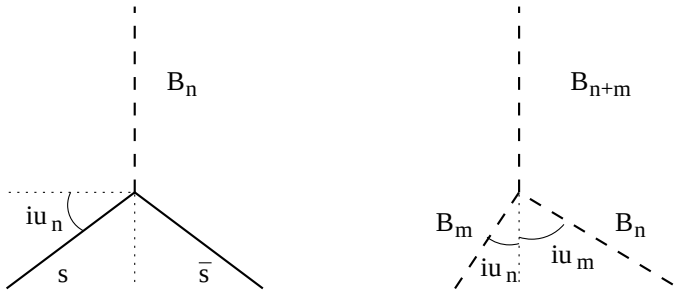


Fig. 25.3. Fusions in the sine-Gordon theory. The soliton and the anti-soliton are represented by full lines, while breathers by dashed lines. All rotated and reflected diagrams are allowed, too.

The scattering of B_n with the soliton $(+)$ or anti-soliton $(-)$ is described compactly by the formula

$$\begin{aligned} S^{+n}_{+n}(\theta) &= S^{-n}_{-n}(\theta) \\ &= \begin{cases} \{n-1+\lambda\}\{n-3+\lambda\}\cdots\{3+\lambda\}\{1+\lambda\} & \text{if } n \text{ is even,} \\ -\{n-1+\lambda\}\{n-3+\lambda\}\cdots\{2+\lambda\}\sqrt{\{\lambda\}} & \text{if } n \text{ is odd,} \end{cases} \end{aligned} \tag{25.39}$$

where we introduced the notation

$$\{y\} \equiv \frac{\left(\frac{y+1}{2\lambda}\right)\left(\frac{y-1}{2\lambda}\right)}{\left(\frac{y+1}{2\lambda}-1\right)\left(\frac{y-1}{2\lambda}+1\right)}, \qquad (x) \equiv -\frac{\sin\left(\frac{\pi x}{2}-\mathrm{i}\frac{\theta}{2}\right)}{\sin\left(\frac{\pi x}{2}+\mathrm{i}\frac{\theta}{2}\right)}. \tag{25.40}$$

Using building block $\{y\}$, which respect the unitarity and are crossing invariant, the breather–breather scatterings can be described as

$$S^{nm}_{nm}(\theta) = \{n+m-1\}\{n+m-3\}\cdots\{|n-m|+3\}\{|n-m|+1\}. \tag{25.41}$$

The spectrum with the soliton, the anti-soliton and the $[\lambda]$ breathers is complete in the sense that all the poles of all scattering matrices can be explained in terms of Coleman-Thun diagrams with nonvanishing couplings, see Fig. 25.3.

25.4.1 Semi-classical limit

We end up this section by the calculation of the soliton and anti-soliton scatterings in the semi-classical $b \to 0$ limit. Supposing that the relation between λ and b takes the form (25.37), we have $\lambda = 8\pi/b^2$ in the leading order. Performing explicitly the $\lambda \to \infty$ limit in the soliton–anti-soliton scatterings, we obtain

$$S^{+-}_{+-}(\theta) \to \exp\left\{\mathrm{i}\frac{8\pi}{b^2}\pi + \mathrm{i}\frac{8\pi}{b^2}\int_0^\infty \frac{\mathrm{d}t}{t^2}\tanh t\,\sinh\left(\frac{2t\theta}{\mathrm{i}\pi}\right)\right\}, \qquad S^{-+}_{+-}(\theta) \to 0. \tag{25.42}$$

These results indicate that the reflection part vanishes and the transmission part is a pure phase shift in the semiclassical limit of the soliton–anti-soliton scattering. This finding is consistent with our classical results in Sect. 22. Let us go beyond the classical limit and compare the

semiclassical phase shift to the classical time shift, encoded in the relation (24.8). The first term shows that the number of bound-states grows as $\frac{8\pi}{b^2}$ in the $b \to \infty$ limit, which is equivalent to the expected $[\lambda]$. The integral in (25.42) can be rewritten as

$$\int_0^\infty \frac{\mathrm{d}t}{t^2}\, \tanh t\, \sin\left(\frac{2t\theta}{\pi}\right) = -\frac{4}{\pi}\int_0^{\tanh(\theta/2)} \mathrm{d}v\, \frac{\ln v}{1-v^2}. \tag{25.43}$$

The velocity of the particles in the center of mass frame is $v = \tanh(\theta/2)$. Thus changing the velocity integral to the energy one, we reproduce exactly the needed result (24.8).

26 UV-IR relation

In the previous sections, we developed consistent quantum frameworks for solving the sine-Gordon theory. Each of these frameworks has different parameters. In the perturbed conformal field theory scheme defined by the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial_t \Phi)^2 - \frac{1}{2}(\partial_x \Phi)^2 - \mu \left(: \mathrm{e}^{\mathrm{i}b\Phi} : + : \mathrm{e}^{-\mathrm{i}b\Phi} : \right), \tag{26.1}$$

the sine-Gordon theory was characterized by the dimensionfull perturbation parameter μ and the dimensionless parameter b, which is the inverse of the compactification radius of the model. We managed to show the existence of higher-spin conserved charges and obtained a numerical spectrum. In the bootstrap quantization, we determined completely the scattering matrix of the soliton and anti-soliton of mass M, in terms of the parameter λ, and in this way we solved the model. It is not clear, however, how the parameters of the two descriptions are related with each other and the aim of the present section is to establish the precise mapping. This is done by calculating the ground-state energy density in the presence of an external field h, coupled to the topological charge, in the two different schemes and by comparing the obtained results [52].

26.1 Ground-state energy density from Perturbed CFT

We study the Euclidean version of the sine-Gordon theory in an external field h, defined by the Lagrangian

$$\begin{aligned} \mathcal{L} &= \mathcal{L}_0 - \mu V_{\mathrm{pert}} \\ &= -\frac{1}{2}(\partial_y \Phi)^2 - \frac{1}{2}(\partial_x \Phi)^2 + h\,\frac{b}{2\pi}\partial_x \Phi - \mu \left(: \mathrm{e}^{\mathrm{i}b\Phi} : + : \mathrm{e}^{-\mathrm{i}b\Phi} : \right). \end{aligned} \tag{26.2}$$

Here, the external field is coupled to the current normalized in such a way that the corresponding topological charge

$$Q = \frac{b}{2\pi}\int_{-\infty}^{\infty} \partial_x \Phi \, \mathrm{d}x \tag{26.3}$$

is equal to 1 for the soliton. We consider the theory on the torus with $x \equiv x + L$ and periodic imaginary time $y \equiv y + R$, with both L and R going to infinity.

Solving the theory for $\mu = 0$ (or, equivalently, in the limit $h \to \infty$), we obtain the equation of motion $\partial_x \Phi = hb/2\pi$ which, according to (23.18), leads to

$$h\frac{b}{2\pi} = \frac{2\pi}{L} r\, m, \qquad r = \frac{1}{b}. \tag{26.4}$$

This shows that the introduced field $hb/(2\pi)$ is quantized in units of $2\pi r/L$ and it merely determines the topological charge of the sector. Since we are interested in the $L \to \infty$ limit, h is basically a continuous variable. The h-dependent part of the ground-state energy density in the sector determined by h is simply

$$e_0 = -\frac{1}{2}\frac{b^2}{4\pi^2}h^2. \tag{26.5}$$

Now we develop a systematic expansion in μ. Recall that the scaling dimension of the perturbing operators is $b^2/(4\pi)$, thus the dimension of the coupling is $[\mu] = 2 - b^2/(4\pi)$. As the dimension of $[h] = 1$ from the dimensional analysis we see that

$$e_0 = -h^2 k(h,\mu) = -h^2 k(\xi), \qquad \xi = \frac{\mu}{h^{2-(b^2/4\pi)}}. \tag{26.6}$$

We see that h works as an infrared cutoff if $\xi \ll 1$. The theory is thus brought to the UV regime in which $k(\xi)$ can be expanded as the Taylor series is ξ,

$$k(\xi) = \sum_{n=0}^{\infty} k_n \xi^n, \qquad k_0 = \frac{b^2}{8\pi^2}, \tag{26.7}$$

where the coefficients k_n can be calculated perturbatively. The ground-state energy density can be extracted from the large-volume asymptotic of the Euclidean partition function

$$Z(L,R) = \mathrm{Tr}\, \mathrm{e}^{-H(L)R} = \mathrm{e}^{-e_0 LR} + \cdots. \tag{26.8}$$

The partition function can be perturbatively evaluated as

$$\begin{aligned} Z[L,R] &= \int [D\Phi]\, \mathrm{e}^{-S[\Phi]} = \int [D\Phi]\, \mathrm{e}^{-S_0[\Phi] - \mu S_{\mathrm{pert}}[\Phi]} \\ &= \int [D\Phi] \sum_{N=1}^{\infty} \frac{(-\mu S_{\mathrm{pert}}[\Phi])^N}{N!} \mathrm{e}^{-S_0[\Phi]} \\ &= \sum_{N=1}^{\infty} \frac{1}{N!} \left\langle (-\mu S_{\mathrm{pert}}[\Phi])^N \right\rangle_0 Z_0(L,R). \end{aligned} \tag{26.9}$$

In the leading non-vanishing order, we have

$$\frac{Z[L,R]}{Z_0[L,R]} = 1 + \frac{\mu^2}{2} \langle S_{\mathrm{pert}}[\Phi] S_{\mathrm{pert}}[\Phi] \rangle_0 + \cdots, \tag{26.10}$$

where the expectation value is evaluated over the unperturbed (conformal) theory in the topological sector prescribed by the external field. The only nonvanishing expectation value is $\langle : \mathrm{e}^{\mathrm{i}b\Phi(x_1,y_1)} :: \mathrm{e}^{-\mathrm{i}b\Phi(x_2,y_2)} : \rangle$ which has to be integrated over both spaces (x_1, y_1) and (x_2, y_2). As the expectation value is translationally invariant, one of the integrations produces the volume factor LR. We calculate the expectation value in the limit $L, R \to \infty$, so the correlation functions on the plane can be used. Keeping in mind that the expectation value is evaluated in the sector m and making the integral dimensionless by introducing the variables $x = b^2 h(x_1 - x_2)/(4\pi)$ and $y = b^2 h(y_1 - y_2)/(4\pi)$, we get

$$\begin{aligned} k_1 &= \left(\frac{b^2}{4\pi}\right)^{b^2/(2\pi)-2} \int (x^2+y^2)^{-b^2/(4\pi)} \mathrm{e}^{-2\mathrm{i}x}\, \mathrm{d}x\, \mathrm{d}y \\ &= \pi \left(\frac{b^2}{4\pi}\right)^{b^2/(2\pi)-2} \frac{\Gamma\left(1 - b^2/(4\pi)\right)}{\Gamma\left(b^2/(4\pi)\right)}. \end{aligned} \tag{26.11}$$

26.2 Ground-state energy from TBA

Now we calculate the h-dependent part of the ground-state energy density in the bootstrap framework, from the scattering matrix, following the method of Ref. [52]. We recall that the spectrum of the sine-Gordon theory contains the soliton and the anti-soliton of mass M and, in dependence on the coupling λ, the breathers B_n $(n = 1, 2, \ldots, [\lambda])$ with masses m_{B_n}. The soliton has the topological charge $Q = 1$, the anti-soliton -1, while the breathers are neutral, i.e. with $Q = 0$. Introducing the external field h, the Hamiltonian will change to

$$H = H_0 - hQ. \tag{26.12}$$

In particular, soliton's energy becomes

$$E(\theta) = M \cosh\theta - h. \tag{26.13}$$

For large enough field $h > M$ the ground-state is no longer the empty state, instead solitons will condense in some field-dependent interval $|\theta| < B(h)$ on the rapidity line. Nice feature of the introduced field h is that it suppresses the influence of other particles to the ground state and keeps only the solitons which scatter diagonally with each other through the S-matrix

$$S_{++}^{++}(\theta) = \mathrm{e}^{-\mathrm{i}\delta(\theta)} = -\exp\left\{\int_0^\infty \frac{\mathrm{d}t}{t}\frac{\sinh(1+\lambda)t}{\sinh t\,\cosh(t\lambda)}\sinh\left(\frac{2\lambda t\theta}{\mathrm{i}\pi}\right)\right\}. \tag{26.14}$$

The rapidities of these solitons are not independent, their interaction is described by Bethe equations. These equation can be heuristically understood as follows. Put N particles with rapidity $\theta_j, j = 1 \ldots N$ in a large volume L. In an integrable field theory, the number of particles is a good quantum number since in the scatterings there is no particle creation and the multiparticle scatterings factorize themselves into pairwise two-particle scatterings. In a finite volume, the momenta and the corresponding energy levels are quantized due to the fact that the multiparticle wave function has to be periodic. Thus when we move a particle around the system size L, we pick up the translation phase $\mathrm{i}pL$ and in addition the scattering phase with all other particles:

$$e^{ip(\theta_j)L}\prod_{k\neq j} S_{++}^{++}(\theta_j - \theta_k) = 1. \tag{26.15}$$

Taking the logarithm of this equation and using the rapidity parameterization of the soliton momentum $p(\theta) = M\sinh(\theta)$, we obtain the usual form of the Bethe equations

$$LM\sinh(\theta_j) - \sum_{k\neq j}\delta(\theta_j - \theta_k) = 2\pi n_j, \qquad n_j \in \mathbb{Z}, \tag{26.16}$$

which are correct up to exponentially small corrections in L. The density of the soliton rapidities is described by the continuous function $\rho(\theta)$ which is reflection symmetric, $\rho(\theta) = \rho(-\theta)$, and nonzero for $\theta \in [-B, B]$ ($B \equiv B(h)$). Since the rapidities are densely packed between $[-B, B]$ for large L, we have $n_j = L\int_0^{\theta_j}\mathrm{d}\theta'\,\rho(\theta')$. Thus, in the thermodynamic limit, the quantization conditions (26.16) simplify to

$$\frac{M}{2\pi}\sinh\theta - \int_{-B}^{B}\frac{\mathrm{d}\theta'}{2\pi}\delta(\theta-\theta')\rho(\theta') = \int_0^\theta \mathrm{d}\theta'\,\rho(\theta'). \tag{26.17}$$

Differentiating this equation with respect to θ, we end up with the integral equation for the soliton density $\rho(\theta)$:

$$\frac{M}{2\pi}\cosh\theta = \rho(\theta) + \int_{-B}^{B} \mathrm{d}\theta' J(\theta-\theta')\rho(\theta'), \qquad J(\theta) = \frac{1}{2\pi}\frac{\partial\delta(\theta)}{\partial\theta}. \tag{26.18}$$

Clearly, because the kernel is negative, $J(\theta) < 0$, the density is discontinuous at B, $\rho(B^-) \neq 0$. For a given $\rho(\theta)$, the ground-state energy density $e_0 = E_0/L$ is written as

$$e_0(h) - e_0(0) = -\int_{-B}^{B} \mathrm{d}\theta\,(h - M\cosh\theta)\rho(\theta). \tag{26.19}$$

The rapidity limit $B(h)$ can be determined by the thermodynamic minimization condition

$$\partial_B e_0(h) = 0. \tag{26.20}$$

As the integral equation (26.18) does not depend explicitly on h, it is better to introduce the energy function $\epsilon(\theta)$ which solves the equation

$$h - M\cosh\theta = \epsilon(\theta) + \int_{-B}^{B} \mathrm{d}\theta'\, J(\theta-\theta')\epsilon(\theta'). \tag{26.21}$$

Plugging back this equation into (26.19) and using Eq. (26.18), we arrive at

$$e_0(h) - e_0(0) = -M\int_{-B}^{B} \frac{\mathrm{d}\theta}{2\pi}\,\cosh\theta\,\epsilon(\theta). \tag{26.22}$$

The advantage of using $\epsilon(\theta)$ instead of $\rho(\theta)$ consists in the fact that the minimization condition (26.20) translates into

$$\epsilon(\pm B) = 0. \tag{26.23}$$

This equality can be obtained by differentiating (26.19) with respect to B and using Eq. (26.21), together with the ∂_B derivative of (26.18).

26.2.1 Leading-order calculation

We are interested in the large-h expansion of $e_0(h)$. There is a standard trick, the so-called dilogarithm trick, how to evaluate the leading-order behaviour of the integral equation (26.21) for large h. Since $\epsilon(\theta)$ is symmetric in θ, we can write

$$e_0(h) = e_0(0) - M\int_{-B}^{B} \frac{\mathrm{d}\theta}{2\pi}\,\mathrm{e}^{\theta}\epsilon(\theta) \approx -M\int_{-\infty}^{B} \frac{\mathrm{d}\theta}{2\pi}\,\mathrm{e}^{\theta}\epsilon(\theta), \tag{26.24}$$

where we used that for large h the integral collects most of the contributions around $\theta \approx B$. In this approximation, the TBA equation (26.21) reduces to

$$h - \frac{M}{2}\mathrm{e}^{\theta} = \epsilon(\theta) + \int_{-\infty}^{B} \mathrm{d}\theta'\, J(\theta-\theta')\epsilon(\theta'). \tag{26.25}$$

After the differentiation with respect to θ and integration by parts, this equation can be put into the form

$$\mathrm{e}^{\theta} = -\frac{2}{M}\left[\epsilon'(\theta) + \int_{-\infty}^{B} \mathrm{d}\theta'\, J(\theta-\theta')\epsilon'(\theta')\right], \qquad \epsilon'(\theta) \equiv \frac{\partial\epsilon(\theta)}{\partial\theta}. \tag{26.26}$$

This equation can be put back into (26.24) to obtain

$$e_0(h) = 2\int_{-\infty}^{B}\int_{-\infty}^{B} \mathrm{d}\theta\,\mathrm{d}\theta'\,\epsilon(\theta)J(\theta-\theta')\epsilon'(\theta') + \frac{1}{\pi}\int_{-\infty}^{B} \mathrm{d}\theta\,\epsilon(\theta)\epsilon'(\theta). \tag{26.27}$$

The θ integration in the first term can be done using (26.25). The subsequent integration by parts leads to

$$e_0(h) = \frac{h}{\pi}\int_{-\infty}^{B} \mathrm{d}\theta\,\epsilon'(\theta) - e_0(h). \tag{26.28}$$

Finally, we arrive at the leading-order result

$$e_0(h) = -\frac{h}{2\pi}\epsilon(-\infty) = -h^2\frac{1}{\pi(\lambda+1)}. \tag{26.29}$$

Here, we used Eq. (26.25) at $\theta = -\infty$ and the explicit form of the kernel. Comparing our result with the conformal perturbative one (26.5) we conclude that

$$\lambda + 1 = \frac{8\pi}{b^2} \tag{26.30}$$

as was anticipated before.

26.2.2 Systematic expansion

In the following part, we solve systematically the TBA integral equation

$$h - M\cosh\theta = \epsilon(\theta) + \int_{-B}^{B} \mathrm{d}\theta'\, J(\theta-\theta')\epsilon(\theta') \equiv \int_{-B}^{B} \mathrm{d}\theta'\, K(\theta-\theta')\epsilon(\theta') \tag{26.31}$$

for large magnetic fields h and calculate the ground-state energy density from $\epsilon(\theta)$. If this linear integral equation were valid on the whole line ($B \to \infty$), we could easily solve it by the Fourier method. The problem consists in extending the equation consistently to the whole line in such a way that we can use the Fourier transformation. For this purpose, we extend the definition of $\epsilon(\theta)$:

$$\epsilon(\theta) = \begin{cases} \epsilon(\theta) & \text{if } |\theta| \le B, \\ 0 & \text{otherwise.} \end{cases} \tag{26.32}$$

The extended TBA equation then takes the form

$$K * \epsilon(\theta) \equiv \int_{-\infty}^{\infty} K(\theta-\theta')\epsilon(\theta')\mathrm{d}\theta' = g(\theta), \tag{26.33}$$

where evidently

$$g(\theta) = h - M\cosh\theta \qquad \text{for } |\theta| \le B. \tag{26.34}$$

However, for $|\theta| > B$, $g(\theta)$ is an unknown function equal to $K * \epsilon$. In Sect. 14, where the unknown function was defined on the half line, we applied the Wiener-Hopf technique to solve this kind of problems. In the present application of the Wiener-Hopf method to a finite interval, we first exploit the $\theta \to -\theta$ symmetry of our problem. Since $K(\theta)$ is symmetric, so is $\epsilon(\theta)$ and we can decompose

$$g(\theta) = Y(\theta) + Y(-\theta) \tag{26.35}$$

with

$$Y(\theta) = \begin{cases} X(\theta) & \text{if } \theta > B, \\ (h - Me^{\theta})/2 & \text{if } \theta \le B. \end{cases} \tag{26.36}$$

The main point of the Wiener-Hopf technique is the unique factorization of the Fourier transform of the kernel into the product of two pieces, one being analytical in the upper and the other in the lower half spaces. In the present case,

$$1 + \hat{J}(\omega) \equiv \hat{K}(\omega) = \int_{-\infty}^{\infty} K(\theta)\mathrm{e}^{\mathrm{i}\omega\theta}\mathrm{d}\theta = \frac{\sinh\frac{\pi\omega(1+\lambda)}{2\lambda}}{2\cosh\frac{\pi\omega}{2}\sinh\frac{\pi\omega}{2\lambda}} \tag{26.37}$$

factorizes into

$$\hat{K}(\omega) = \frac{1}{\hat{K}_+(\omega)\hat{K}_-(\omega)}, \tag{26.38}$$

where

$$\hat{K}_-(\omega) = \sqrt{2\pi(1+\lambda)}\frac{\Gamma(\mathrm{i}\frac{1+\lambda}{2\lambda}\omega)}{\Gamma(\mathrm{i}\frac{\omega}{2\lambda})\Gamma(\frac{1}{2}+\mathrm{i}\frac{\omega}{2})}\mathrm{e}^{\mathrm{i}\omega\Delta}; \qquad \hat{K}_+(\omega) = \hat{K}_-(-\omega) \tag{26.39}$$

and

$$\Delta = \frac{1}{2}\ln\lambda - \frac{(1+\lambda)}{2\lambda}\ln(1+\lambda). \tag{26.40}$$

As required, $\hat{K}_+(\omega)$ is analytical in the upper, while $\hat{K}_-(\omega)$ in the lower half planes. The asymptotic of $\hat{K}_+(\omega) = 1 + O(1/\omega)$ holds everywhere, except on the negative imaginary axis where its poles and zeros are located. In particular, this means that $\hat{K}_+(\omega) - 1 \equiv \hat{k}_+(\omega)$ is analytical in the upper half plane and has a vanishing asymptotic there. As a consequence, the function

$$k_+(\theta) = \int_{-\infty}^{\infty} \hat{k}_+(\omega)\mathrm{e}^{-\mathrm{i}\omega\theta}\frac{\mathrm{d}\omega}{2\pi} \tag{26.41}$$

is vanishing for $\theta < 0$. Similar findings apply to $\hat{K}_+(\omega)^{-1} - 1$. Analogously, $\hat{K}_-(\omega) - 1 \equiv \hat{k}_-(\omega)$ is analytical in the lower half plane and has vanishing asymptotic there. Hence $k_-(\theta)$ is vanishing for $\theta > 0$, just as the inverse Fourier transform of $\hat{K}_-(\omega)^{-1} - 1$.

The TBA equation has the formal solution

$$\hat{\epsilon}(\omega) = \hat{K}_+(\omega)\hat{K}_-(\omega)\left[\hat{Y}(\omega) + \hat{Y}(-\omega)\right]. \tag{26.42}$$

In analogy with Sect. 14, we divide both sides of this relation by $\hat{K}_-(\omega)$ and analyze their analytical structure:

$$\hat{K}_-(\omega)^{-1}\hat{\epsilon}(\omega) = \hat{K}_+(\omega)\hat{Y}(\omega) + \hat{K}_-(-\omega)\hat{Y}(-\omega)). \tag{26.43}$$

In the coordinate space, this equation reads as

$$K_-^{-1} * \epsilon\,(\theta) = K_+ * Y\,(\theta) + K_- * Y\,(-\theta). \tag{26.44}$$

Unfortunately, $\epsilon(\theta)$ is nonvanishing on the interval $[-B, B]$ and not on the positive line like the functions in Sect. 14. This is why we define the operations $[\cdots]_\pm$ which project the positive and negative "parts" of a function in the following way

$$[f(\theta)]_+ = \begin{cases} f(\theta) & \text{if } \theta > B, \\ 0 & \text{if } \theta < B, \end{cases} \qquad [f(\theta)]_- = \begin{cases} 0 & \text{if } \theta > B, \\ f(\theta) & \text{if } \theta < B. \end{cases} \tag{26.45}$$

It can be shown that the Fourier transform of these functions can be expressed by using $\hat{f}(\omega)$ as follows

$$\hat{[f]}_\pm(\omega) = \mp \mathrm{e}^{\mathrm{i}\omega B} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\omega' B}\hat{f}(\omega')}{\omega - \omega' \pm \mathrm{i}0} \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \tag{26.46}$$

Using that the inverse Fourier transform of $\hat{K}_-(\omega)^{-1} - 1$ is nonvanishing for negative θ only, we get

$$\left[K_-^{-1} * \epsilon\,(\theta)\right]_+ = 0. \tag{26.47}$$

In the view of Eq. (26.44), this is equivalent to

$$[K_+ * Y\,(\theta)]_+ = -\,[K_- * Y\,(-\theta)]_+ \tag{26.48}$$

and we have eliminated ϵ from the formalism. Using that $f(\theta) = [f(\theta)]_+ + [f(\theta)]_-$, we derive an integral equation for $Y(\theta)$ from

$$K_+ * Y\,(\theta) = [K_+ * Y\,(\theta)]_- - [K_- * Y\,(-\theta)]_+\,. \tag{26.49}$$

Fortunately we are able to calculate explicitly $[K_+ * Y(\theta)]_-$. Since $K_+ - 1$ is nonvanishing only for $\theta > 0$ and $Y(\theta) = (h - M\mathrm{e}^\theta)/2$ only for $\theta \le B$, we have

$$[K_+ * Y\,(\theta)]_- = \begin{cases} 0 & \text{if } \theta > B, \\ \left[\hat{K}_+(0)h - \hat{K}_+(\mathrm{i})M\mathrm{e}^\theta\right]/2 & \text{if } \theta < B. \end{cases} \tag{26.50}$$

It is more convenient to rewrite the integral equation (26.49) in the Fourier space, in terms of the unknown function

$$\hat{v}(\omega) = \mathrm{e}^{-\mathrm{i}\omega B}\hat{K}_+(\omega)\hat{Y}(\omega). \tag{26.51}$$

We find that this function is determined by

$$\hat{v}(\omega) = -\frac{\mathrm{i}h\hat{K}_+(0)}{2(\omega - \mathrm{i}0)} + \frac{\mathrm{i}M\mathrm{e}^B\hat{K}_+(\mathrm{i})}{2(\omega - i)} + \int_{-\infty}^{\infty} \frac{\mathrm{e}^{2\mathrm{i}\omega' B}}{\omega + \omega' + \mathrm{i}0} \frac{\hat{K}_-(\omega')}{\hat{K}_+(\omega')} \hat{v}(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \tag{26.52}$$

It is useful to deform the integration contour to encircle the singularities of the integrated functions $\hat{v}(\omega)$ and $\hat{K}_-(\omega)/\hat{K}_+(\omega)$. Except for the explicit simple poles at 0 and i, they are all located on the positive imaginary axis. Picking up the singularity at 0, we obtain

$$\hat{v}(\omega) = -\frac{\mathrm{i}h\hat{K}_+(0)}{\omega} + \frac{\mathrm{i}M\mathrm{e}^B\hat{K}_+(\mathrm{i})}{2(\omega - \mathrm{i})} + \int_{C_+} \frac{\mathrm{e}^{2\mathrm{i}\omega' B}}{\omega + \omega'} \frac{\hat{K}_-(\omega')}{\hat{K}_+(\omega')} \hat{v}(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}, \tag{26.53}$$

where now the integration goes around the positive imaginary axis, leaving the origin out. Once we determined $\hat{v}(\omega)$ we can calculate $\hat{\epsilon}(\omega)$ from (26.42):

$$\hat{\epsilon}(\omega) = \mathrm{e}^{\mathrm{i}\omega B}\hat{K}_-(\omega)\hat{v}(\omega) + \mathrm{e}^{-\mathrm{i}\omega B}\hat{K}_+(\omega)\hat{v}(-\omega). \tag{26.54}$$

Explicitly, we have

$$\frac{\mathrm{e}^{-\mathrm{i}\omega B}\hat{\epsilon}(\omega)}{\hat{K}_-(\omega)} = -\frac{\mathrm{i}h\hat{K}_+(0)}{\omega} + \frac{\mathrm{i}M\mathrm{e}^B\hat{K}_+(\mathrm{i})}{2(\omega - \mathrm{i})} + \int_{C'_+} \frac{\mathrm{e}^{2\mathrm{i}\omega' B}}{\omega + \omega'} \frac{\hat{K}_-(\omega')}{\hat{K}_+(\omega')} \hat{v}(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}, \tag{26.55}$$

where in the integration the pole at $\omega' = -\omega$ has to be surrounded, too. Finally, the change in the ground-state energy (26.22) can be expressed as

$$\begin{aligned} e_0(h) - e_0(0) = -\frac{M}{2\pi}\hat{\epsilon}(-\mathrm{i}) \quad &= \quad -\frac{M\mathrm{e}^B}{2\pi}\hat{K}_+(\mathrm{i}) \Bigg[h\hat{K}_+(0) - \frac{M\mathrm{e}^B}{4}\hat{K}_+(\mathrm{i}) \\ &\qquad + \int_{C'_+} \frac{\mathrm{e}^{2\mathrm{i}\omega' B}}{\omega' - \mathrm{i}} \frac{\hat{K}_-(\omega')}{\hat{K}_+(\omega')} \hat{v}(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}} \Bigg]. \end{aligned} \tag{26.56}$$

We are left with the boundary condition $\epsilon(\pm B) = 0$. In the language of $\hat{v}(\omega)$, this condition requires the asymptotic behaviour $\hat{v}(\omega) = O(1/\omega^2)$ and, consequently, the cancellation of the leading $O(1/\omega)$ terms in the integral equation (26.53):

$$\mathrm{i}h\hat{K}_+(0) - \frac{\mathrm{i}M}{2}\mathrm{e}^B\hat{K}_+(\mathrm{i}) = \int_{C_+} \mathrm{e}^{2\mathrm{i}\omega' B} \frac{\hat{K}_-(\omega')}{\hat{K}_+(\omega')} \hat{v}(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}. \tag{26.57}$$

In order to develop the large-h expansion, we simplify the notation by introducing

$$u(\omega) = -\frac{1 + \mathrm{i}\omega}{h\hat{K}_+(0)}\hat{v}(\omega), \qquad \rho(\omega) = \frac{1 - \mathrm{i}\omega}{1 + \mathrm{i}\omega} \frac{\hat{K}_-(\omega)}{\hat{K}_+(\omega)}. \tag{26.58}$$

With these functions the integral equation can be transformed into the form

$$u(\omega) = \frac{\mathrm{i}}{\omega} + \int_{C_+} \frac{\mathrm{e}^{2\mathrm{i}\omega' B}}{\omega + \omega'} \rho(\omega') u(\omega') \frac{\mathrm{d}\omega'}{2\pi\mathrm{i}} \tag{26.59}$$

and the boundary condition $\epsilon(\pm B) = 0$ leads to

$$u(\mathrm{i}) = y^{\frac{1+\lambda}{4\lambda}} \mathrm{e}^{B+\Delta}, \qquad y = \left[\frac{M\sqrt{\pi}(1+\lambda)}{2h} \frac{\Gamma(\frac{1+\lambda}{2\lambda})}{\Gamma(\frac{1}{2\lambda})} \right]^{4\lambda/(1+\lambda)}. \tag{26.60}$$

This is the very equation which relates the rapidity limit B to the magnetic field h. Once the function $u(\omega)$ is determined, the change of the specific ground-state energy density due to the field can be written as

$$e_0(\mu, h) - e_0(\mu, 0) = -\frac{h^2 u(\mathrm{i})}{\pi(1+\lambda)} \left[1 - \int_{C_+} \frac{\mathrm{e}^{2\mathrm{i}\omega B}}{\omega - \mathrm{i}} \rho(\omega) u(\omega) \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \right]. \tag{26.61}$$

We identify $e_0(\mu, h = 0)$ as the h-independent part of the rhs. It comes from the explicit pole at $\omega = \mathrm{i}$:

$$e_0(\mu, h = 0) \equiv e_0(\mu) - e_0|_{\mathrm{free}} = -\frac{M^2}{4} \tan\left(\frac{\pi}{2\lambda}\right), \tag{26.62}$$

where $e_0|_{\mathrm{free}} = e_0(\mu = 0)$ is the specific ground-state energy of the free model.

It is instructive to evaluate the underlying integrals by using the residue theorem. Besides the explicit pole at i, which was already analyzed, there are another poles at $\omega_n = 2\mathrm{i}n\lambda/(1+\lambda)$ $(n = 1, 2, \ldots)$. The residues of the kernel-related function ρ at ω_n can be calculated explicitly, with the result

$$b_n \equiv \frac{\mathrm{i}(1+\lambda)}{2\lambda} \mathrm{e}^{4n\Delta\lambda/(1+\lambda)} \mathrm{res}_{\omega=\omega_n} \rho(\omega) = \frac{(-1)^n}{n!(n-1)!} \frac{\Gamma(\frac{n}{1+\lambda})\Gamma(\frac{3}{2} + \frac{n\lambda}{1+\lambda})}{\Gamma(-\frac{n}{1+\lambda})\Gamma(\frac{3}{2} - \frac{n\lambda}{1+\lambda})}. \tag{26.63}$$

From Eq. (26.59) we obtain a coupled set of equations for $w_n = 2\lambda u(\omega_n)/(1+\lambda)$:

$$w_n = \frac{1}{n} - \sum_{m=1}^{\infty} \frac{q^m}{m+n} b_m w_m, \qquad q = \exp\left(-\frac{4[B+\Delta]\lambda}{1+\lambda} \right). \tag{26.64}$$

The boundary condition (26.60) relates q to the magnetic field h as follows

$$y = q \left(1 - \sum_{n=1}^{\infty} \frac{1+\lambda}{1+(2n+1)\lambda} q^n b_n w_n \right)^{4\lambda/(1+\lambda)}. \tag{26.65}$$

Finally, the ground-state energy density can be expressed as $e_0(h) = -h^2 k(h, M)$ with

$$\begin{aligned} k(h, M) &= \frac{1}{1+\lambda} \left(1 - \sum_{n=1}^{\infty} \frac{1+\lambda}{1+(1+2n)\lambda} q^n b_n w_n \right) \\ &\quad \times \left(1 - \sum_{n=1}^{\infty} \frac{1+\lambda}{1+(1-2n)\lambda} q^n b_n w_n \right). \end{aligned} \tag{26.66}$$

Note that the limit $q \to 0$ corresponds to $B \gg 1$ (large magnetic field, UV regime). The above systems of equations can be solved iteratively in powers of q, which can be translated via Eq. (26.65) into an expansion in y:

$$k(h, M) = \sum_{n=0}^{\infty} K_n y^n. \tag{26.67}$$

The first two coefficients are obtained in the form

$$K_0 = \frac{1}{\pi(1+\lambda)}, \qquad K_1 = -\frac{2b_1(1+\lambda)}{\pi(1-\lambda)(1+3\lambda)}. \tag{26.68}$$

Now we make a comparison with the previous UV expansion (26.6). With regard to the relation (26.30), the first coefficient K_0 is nothing but the leading-order coefficient k_0 calculated previously. The next coefficient, however, after identifying $k_1\xi = K_1 y$ with k_1 given by (26.11), implies the explicit relation between the Lagrangian parameter μ and the soliton mass M:

$$\mu = \frac{1}{\pi}\frac{\Gamma\left(\frac{1}{1+\lambda}\right)}{\Gamma\left(\frac{\lambda}{1+\lambda}\right)}\left[M\frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{1+\lambda}{2\lambda}\right)}{\Gamma\left(\frac{1}{2\lambda}\right)}\right]^{2\lambda/(1+\lambda)}. \tag{26.69}$$

27 Exact finite volume description from XXZ

In Sect. 17, the thermodynamics of the XXZ Heisenberg chain was analyzed using the quantum transfer matrix. The weights of the S-matrix in (17.3) were chosen as

$$a(u) = 1, \qquad b(u) = -\frac{\sin(\gamma u/2)}{\sin(\gamma + \gamma u/2)}, \qquad c(u) = \frac{\sin(\gamma)}{\sin(\gamma + \gamma u/2)}, \tag{27.1}$$

where we modified the notation of the rapidity from λ to u, γ is a parameter of the lattice model and the minus sign added to b does not change the partition function (which depends on b^2). It was shown that the free energy per site can be calculated from the $N \to \infty$ limit of the largest eigenvalue of the alternating quantum transfer matrix (17.12). In Sect. 17.3, two nonlinear integral equations were derived for the eigenvalues of the quantum transfer matrix. Interestingly, these equations contain the kernel [see Eq. (17.57)]

$$p(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{\sinh\left(\frac{\pi}{\gamma} - 2\right) k}{2\cosh k \, \sinh\left(\frac{\pi}{\gamma} - 1\right) k} \mathrm{e}^{\mathrm{i}kx}, \tag{27.2}$$

which is trivially related to the logarithmic derivative of the soliton-soliton scattering matrix $S_{++}^{++}(\theta)$, if the identifications $\pi/\gamma - 1 = \lambda^{-1}$ and $x = 2\theta/\pi$ are made. Notice however that the first identification differs from the one $\pi/\gamma = \lambda^{-1}$ obtained from the comparison of the S-matrices (25.27) and (27.1) themselves. Nevertheless, there is a hope that the continuum limit of the XXZ model is related to the sine-Gordon theory, although the parameters may be renormalized.

The continuum limit of the XXZ model is the free boson $c = 1$ conformal field theory. In order to describe its massive perturbation, we have to introduce a mass scale in the lattice model. This can be done either by analyzing the XYZ model [54], or by introducing alternating inhomogeneities into the XXZ model, as was done in the quantum transfer matrix approach. There the inhomogeneity τ depends on the Trotter number N like $\tau \propto N^{-1}$ and vanishes in the $N \to \infty$ limit. In order to describe a massive theory we have to choose τ to be imaginary and send it to infinity in such a way that the resulting source term [see Eq. (26.16)] and the integral equation [see Eq. (17.58)] become

$$-\mathrm{i} \ln \mathrm{a}(x) = ML \sinh \frac{\pi x}{2} + \omega + 2 \int_{-\infty}^{\infty} \mathrm{d}x' \, p(x - x') \Im m \, \ln[1 + \mathrm{a}(x' + \mathrm{i}0)]. \tag{27.3}$$

Here, ω represents a twisted boundary condition which originates from the magnetic field in the XXZ model. The function $\mathrm{a}(x)$ is related to the ground state of the system. Within this description the continuum sine-Gordon theory in volume L is obtained as a continuum limit of an alternating light-cone XXZ spin chain and its energy can be read off from $\mathrm{a}(x)$ by using the relation

$$E_0(L) = -2M \int_{-\infty}^{\infty} \mathrm{d}x \, \sinh\left(\frac{\pi x}{2}\right) \Im m \, \ln[1 + \mathrm{a}(x + \mathrm{i}0)]. \tag{27.4}$$

Thus the same kind of integral equations, with different source terms, describe the ground-state energy of the XXZ model in a magnetic field, as well as its thermodynamics, and the sine-Gordon

ground-state energy in finite volume L [53]. In the following part we document how the same integral equation, but with more general source terms, can describe all states of the sine-Gordon theory in finite volume.

27.1 Excited states from the lattice

We indicated that the ground-state energy of the sine-Gordon model can be described by taking a double scaled limit of the alternating XXZ spin chain. In the following, we derive integral equations for excited states of the sine-Gordon model by analyzing the states close to the antiferromagnetic vacuum of the spin chain.

We aim at analyzing an alternating XXZ spin chain with inhomogeneities $(-1)^n\Theta$. For this purpose we rescale u to $\theta = \mathrm{i}u\pi/2$ and introduce weights which are closer to the sine-Gordon S-matrix,

$$a(\theta) = 1, \qquad b(\theta) = \frac{\sin\left(\mathrm{i}\frac{\gamma}{\pi}\theta\right)}{\sin\frac{\gamma}{\pi}(\pi + \mathrm{i}\theta)}, \qquad c(\theta) = \frac{\sin\gamma}{\sin\frac{\gamma}{\pi}(\pi + \mathrm{i}\theta)}. \tag{27.5}$$

The quantum transfer matrix is similar to that in (17.12), except for we use the same S-matrix everywhere (instead of $\tilde{S}$):

$$T(\theta)^{\sigma_1\dots\sigma_N}_{\sigma'_1\dots\sigma'_N} = \sum_{\{\gamma\}}\prod_{n=1}^{N/2} S^{\sigma_{2n-1}\gamma_{2n-1}}_{\sigma'_{2n-1}\gamma_{2n}}(\theta-\Theta)S^{\sigma_{2n}\gamma_{2n}}_{\sigma'_{2n}\gamma_{2n+1}}(\theta+\Theta). \tag{27.6}$$

We are interested in the eigenvectors and eigenvalues of this matrix. They can be characterized by the roots $\{\theta_j\}_{j=1}^M$ which satisfy the Bethe ansatz equations

$$\frac{q(\theta_j + \mathrm{i}\pi)}{q(\theta_j - \mathrm{i}\pi)} = -\frac{\phi(\theta_j + \frac{\mathrm{i}\pi}{2})}{\phi(\theta_j - \frac{\mathrm{i}\pi}{2})}. \tag{27.7}$$

Here, in analogy with Sect. 17,

$$q(\theta) = \prod_{j=1}^{M} r(\theta - \theta_j), \quad r(\theta) = \sinh\left(\frac{\gamma}{\pi}\theta\right), \quad \phi(\theta) = \left[r(\theta+\Theta)r(\theta-\Theta)\right]^{N/2}. \tag{27.8}$$

Light-cone components of the energy and momentum can be deduced from the transfer matrix as follows

$$\mathrm{e}^{\mathrm{i}a(E\pm P)} = (-1)^M \frac{q\left(\pm(\Theta + \frac{\mathrm{i}\pi}{2})\right)}{q\left(\pm(\Theta - \frac{i\pi}{2})\right)}, \tag{27.9}$$

where the lattice spacing $a = L/N$ is sent to zero.

We can introduce the function

$$\mathrm{a}(\theta) = \frac{q(\theta + \mathrm{i}\pi)\phi\left(\theta - \frac{\mathrm{i}\pi}{2}\right)}{q(\theta - \mathrm{i}\pi)\phi\left(\theta + \frac{\mathrm{i}\pi}{2}\right)} \tag{27.10}$$

such that

$$\mathrm{a}(\theta_j) = -1 \tag{27.11}$$

whenever θ_j is a Bethe root. In the ground state, all Bethe roots θ_j are real and we can use, similarly to Sect. 17.3, the derivative of $\ln(1+\mathrm{a}(\theta))$ to reformulate the BA equations by integrating around the real line.

For excited states complex Bethe roots appear as well. Those roots, whose imaginary part satisfies

$$|\Im m(\theta_j)| < \min(\pi, \pi-\gamma) \tag{27.12}$$

are called close roots. We denote the close roots by θ_j^c and their number by N_C. The remaining complex roots, which do not satisfy the above inequality, are called wide roots. They are denoted by θ_j^w and their number by N_W. Clearly, the Bethe ansatz is periodic with period $\mathrm{i}\pi^2/\gamma$, thus we can restrict ourselves to $|\Im m(\theta_j^w)| < \pi^2/(2\gamma)$. Analyzing excited states, we may find real positions θ_j^h such that the condition $\mathrm{a}(\theta_j^h) = -1$ is satisfied, but θ_j^h is not a Bethe root. Such positions are called holes and their number is denoted by N_H. In order to use the methods of Sect. 17.3, we rewrite $\mathrm{a}(\theta)$ as

$$\mathrm{a}(\theta)\frac{q_c(\theta-\mathrm{i}\pi)}{q_c(\theta+\mathrm{i}\pi)}\frac{q_w(\theta-\mathrm{i}\pi)}{q_w(\theta+\mathrm{i}\pi)}\frac{q_h(\theta+\mathrm{i}\pi)}{q_h(\theta-\mathrm{i}\pi)} = \frac{\tilde{q}(\theta+\mathrm{i}\pi)\phi\left(\theta-\frac{\mathrm{i}\pi}{2}\right)}{\tilde{q}(\theta-\mathrm{i}\pi)\phi\left(\theta+\frac{\mathrm{i}\pi}{2}\right)} = \tilde{\mathrm{a}}(\theta), \tag{27.13}$$

where a is defined by (27.10), i.e. it contains the contributions of real roots and

$$q_c(\theta) = \prod_{j=1}^{N_C} r(\theta-\theta_j^c), \quad q_w(\theta) = \prod_{j=1}^{N_W} r(\theta-\theta_j^w), \quad q_h(\theta) = \prod_{j=1}^{N_H} r(\theta-\theta_j^h) \tag{27.14}$$

and $\tilde{q}(\theta) = q(\theta)q_h(\theta)$ was chosen such that $1+\tilde{\mathrm{a}}(\theta) = 0$ is satisfied only for the real roots, i.e. $\tilde{\mathrm{a}}(\theta)$ behaves like $\mathrm{a}(\theta)$ behaved in the vacuum. Using a derivation analogous to Sect. 17, we obtain

$$\begin{aligned} -\mathrm{i}\ln\,\mathrm{a}(\theta) &= 2N\arctan\left(\frac{\sinh\theta}{\cosh\Theta}\right) + g(\theta|\{\theta_j\}) \\ &\quad +2\Im m\int_{-\infty}^{\infty}\mathrm{d}\theta'\,p\left(\frac{2}{\pi}(\theta-\theta')\right)\ln\left[1+\mathrm{a}(\theta+\mathrm{i}0)\right], \end{aligned} \tag{27.15}$$

where $g(\theta|\{\theta_j\})$ comes from q_c, q_w and q_h as will be explained later. Note that the lattice spacing appears only in the source term, see also Eq. (17.50). In the lattice model, we have as parameters the anisotropy γ, the inhomogeneity Θ and the size N. Taking the continuum limit we should match these parameters to that of the sine-Gordon theory, namely to the parameter λ, the mass parameter M and the volume L. In order to describe a relativistically invariant continuum theory with mass M we take $N\to\infty$ in such a way that $\Theta\to\infty$ as

$$\Theta = \ln\left(\frac{4N}{ML}\right). \tag{27.16}$$

In this limit the source term becomes $ML\sinh\theta$ and we obtain the integral equation which determines the energy of a given state in the sine-Gordon theory in volume L, where $\pi/\gamma - 1 = \lambda^{-1}$.

27.2 Integral equation for the spectrum

To make connection to the literature, we introduce instead of $\mathrm{a}(\theta)$ the new functions $Z(\theta) = -\mathrm{i}\ln[(-1)^\delta \mathrm{a}(\theta)]$, where $\delta = 0, 1$ (the origin of δ comes from the lattice and encodes the parity of the number of magnons in the given state). The integral equation is transformed to

$$\begin{aligned} Z(\theta) &= ML\sinh\theta + g(\theta|\{\theta_j\}) \\ &\quad +2\Im m\int_{-\infty}^{\infty}\mathrm{d}\theta'\, G(\theta-\theta'-\mathrm{i}\eta)\ln\left[1+(-1)^\delta \mathrm{e}^{\mathrm{i}Z(\theta'+\mathrm{i}\eta)}\right], \end{aligned} \tag{27.17}$$

where $\eta > 0$ is a small parameter, of which the result is independent, and

$$G(\theta) = p\left(\frac{2\theta}{\pi}\right) = \int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}\frac{\sinh(1-\lambda)\frac{k}{\lambda}}{2\cosh k\,\sinh\frac{k}{\lambda}}\mathrm{e}^{\mathrm{i}2k\theta/\pi}. \tag{27.18}$$

The source terms are given by

$$g(\theta|\{\theta_j\}) = \sum_{k=1}^{N_H}\chi(\theta-\theta_k^h) - \sum_{k=1}^{N_C}\chi(\theta-\theta_k^c) - \sum_{k=1}^{N_W}\chi_{II}(\theta-\theta_k^w) \quad , \tag{27.19}$$

where

$$\chi(\theta) = 2\pi\int_0^\theta \mathrm{d}\theta'\, G(\theta') \tag{27.20}$$

is the soliton-soliton scattering phase (modulo $\mathrm{i}\pi$). The sine-Gordon theory behaves quite differently in the repulsive ($\lambda < 1$) and attractive ($\lambda > 1$) regimes. This can be seen also from the kernel (27.18). When we analytically continue any function along the imaginary direction, the line $\min(\pi, \pi/\lambda)$ plays an important role. The domain above this line is called the second determination and for any function its analytically continued function is

$$f_{II}(\theta) = \begin{cases} f(\theta) + f(\theta - \mathrm{i}\pi\,\mathrm{sign}(\Im m(\theta))) & \text{for } \lambda < 1, \\ f(\theta) - f(\theta - \mathrm{i}\frac{\pi}{\lambda}\,\mathrm{sign}(\Im m(\theta))) & \text{for } \lambda > 1, \end{cases} \tag{27.21}$$

whenever $|\Im m(\theta)| > \min(\pi, \pi/\lambda)$. The source positions are determined from the Bethe quantization conditions

$$Z(\theta_j) = 2\pi I_j, \qquad I_j \in \mathbb{Z} + \frac{1-\delta}{2}. \tag{27.22}$$

Given a solution for Z, the energy and momentum can be calculated from

$$\begin{aligned} E &= e_0 L + M\sum_{k=1}^{N_H}\cosh\theta_k^h - M\sum_{k=1}^{N_C}\cosh\theta_j^c - M\sum_{k=1}^{N_W}\cosh_{II}\theta_k^w \\ &\quad -2M\Im m\int_{-\infty}^{\infty}\mathrm{d}\theta\,\sinh(\theta+\mathrm{i}\eta)\ln\left[1+(-1)^\delta\mathrm{e}^{\mathrm{i}Z(\theta+\mathrm{i}\eta)}\right], \end{aligned} \tag{27.23}$$

$$\begin{aligned} P &= M\sum_{k=1}^{N_H}\sinh\theta_k^h - M\sum_{k=1}^{N_C}\sinh\theta_j^c - M\sum_{k=1}^{N_W}\sinh_{II}\theta_k^w \\ &\quad -2M\Im m\int_{-\infty}^{\infty}\mathrm{d}\theta\,\cosh(\theta+\mathrm{i}\eta)\ln\left[1+(-1)^\delta\mathrm{e}^{\mathrm{i}Z(\theta+\mathrm{i}\eta)}\right]. \end{aligned} \tag{27.24}$$

Here, we introduced the ground-state energy density e_0 (26.62) by hand, to be comparable with the perturbed conformal field theory.

Finally we note that the characterization of holes and roots is complete for large volumes only. For small volumes the so-called special objects can appear, which modify the formulas above. For example, one has to use the effective hole number $N_H^{\text{eff}} = N_H - 2N_S$; for details see [41]. As the topological charge can be identified as twice the spin of the Heisenberg chain, we obtain the relation

$$Q = 2S = \begin{cases} N_H - N_C & \text{for } \lambda > 1, \\ N_H - N_C - 2N_W & \text{for } \lambda < 1. \end{cases} \tag{27.25}$$

27.3 Large volume expansion

In order to compare the integral equation with the scattering theory, first we analyze the large volume expansion. The integral equation (27.17) can be solved iteratively in the large volume limit. In leading order, we can drop the integral term and write

$$Z(\theta) = ML\sinh\theta + \sum_{k=1}^{N_H} \chi(\theta - \theta_k^h) - \sum_{k=1}^{N_C} \chi(\theta - \theta_k^c) - \sum_{k=1}^{N_W} \chi_{II}(\theta - \theta_k^w). \tag{27.26}$$

In order to see how good is this approximation we can plug this solution back into (27.17). In the integral term we can shift η until we reach some singularity. This singularity can occur at $\mathrm{i}\pi/2$ for $\lambda < 1$ and $\mathrm{i}\pi/(2\lambda)$ for $\lambda > 1$. The corrections in these cases are of order $\exp(-ML\cosh\theta)$ and $\exp(-2ML\sin(\pi/2\lambda)\cosh\theta)$, respectively. Thus, up to exponentially small corrections in the volume, it is sufficient to consider the leading order result (27.26). First we focus on excited states composed exclusively of holes, afterwards we analyze other roots separately for the repulsive and attractive regimes.

If we have only holes θ_j^h for $j = 1 \dots N_H$, the quantization condition takes the form

$$(-1)^\delta e^{\mathrm{i}Z(\theta_j^h)} = (-1)^{\delta - N_H} \mathrm{e}^{\mathrm{i}ML\sinh\theta_j^h} \prod_{k:k\neq j} S_{++}^{++}(\theta_j^h - \theta_k^h) = 1, \tag{27.27}$$

once we used that

$$\mathrm{e}^{\mathrm{i}\chi(\theta)} = -S_{++}^{++}(\theta), \qquad \chi(0) = 0. \tag{27.28}$$

The equation (27.27) is the momentum quantization condition for N_H solitons in volume L if $\delta = N_H \bmod 2$. Thus the θ_j^h locations can be interpreted as the rapidities of the solitons. This interpretation is also supported by the energy and momentum formulas which in the leading order read

$$E = e_0 L + M\sum_{k=1}^{N_H} \cosh\theta_k^h, \qquad P = M\sum_{k=1}^{N_H} \sinh\theta_k^h. \tag{27.29}$$

Consequently the solitons can be viewed as holes in the infinite see of Bethe roots formed in the termodynamic limit of the XXZ model [55, 56].

27.3.1 Repulsive regime

Here we analyze scattering states in the repulsive $\lambda < 1$ regime [57]. Let us start with two-particle states. A two-soliton scattering state can be described by two holes θ_1^h and θ_2^h. According to (27.25), the corresponding topological charge is equal to 2. As the parity is the symmetry of the system even in finite volume, the same integral equation describes the state with two anti-solitons. The description of the sector of the zero topological charge is more complicated because in the scattering the $s(\theta_1)\bar{s}(\theta_2)$ state is mixed with the $\bar{s}(\theta_1)s(\theta_2)$ state. Thus we have to diagonalize the scattering matrix

$$\begin{aligned}\begin{pmatrix} S_{+-}^{+-}(\theta) & S_{+-}^{-+}(\theta) \\ S_{-+}^{+-}(\theta) & S_{-+}^{-+}(\theta) \end{pmatrix} \quad &\longrightarrow \quad \begin{pmatrix} S_+(\theta) & 0 \\ 0 & S_-(\theta) \end{pmatrix} \\ &= \quad \begin{pmatrix} -\frac{\sinh\lambda(\theta+\mathrm{i}\pi)/2}{\sinh\lambda(\theta-\mathrm{i}\pi)/2} & 0 \\ 0 & \frac{\cosh\lambda(\theta+\mathrm{i}\pi)/2}{\cosh\lambda(\theta-\mathrm{i}\pi)/2} \end{pmatrix} S_{++}^{++}(\theta) \end{aligned} \tag{27.30}$$

and to use the quantization condition

$$\mathrm{e}^{\mathrm{i}ML\sinh\theta_1} S_\pm(\theta_1-\theta_2) = 1, \qquad \mathrm{e}^{\mathrm{i}ML\sinh\theta_2} S_\pm(\theta_2-\theta_1) = 1 \tag{27.31}$$

in the two cases. This is what we recover from the integral equation (27.17).

Careful investigation shows that the symmetric solution (S_+) can be described by two holes θ_1^h and θ_2^h and a pair of close complex-conjugate roots $\frac{1}{2}(\theta_1^h+\theta_2^h) \pm \mathrm{i}\frac{\pi-\epsilon}{2}$, where for large volume ϵ is exponentially small. Evaluating $Z(\theta)$ at θ_1^h and θ_2^h yields (27.31). The energy and momentum are given by

$$E = M\cosh\theta_1^h + M\cosh\theta_2^h, \qquad P = M\sinh\theta_1^h + M\sinh\theta_2^h. \tag{27.32}$$

The simple representation is due to the special location of the complex roots, namely their difference is $\mathrm{i}\pi$. The topological charge of the state is $Q = N_H - N_C = 2-2 = 0$, as was expected.

The antisymmetric solution of the two particle state (S_-) can be obtained by creating two holes at θ_1^h and θ_2^h and a single self-conjugate wide root at $\frac{1}{2}(\theta_1^h+\theta_2^h) + \mathrm{i}\frac{\pi}{2\lambda}(1+\lambda)$. This root decreases the topological charge by 2, but does not change the energy and momentum since it holds

$$\cosh_{II}\theta = \cosh\theta + \cosh(\theta-\mathrm{i}\pi) = 0, \ \sinh_{II}\theta = \sinh\theta + \sinh(\theta-\mathrm{i}\pi) = 0 \tag{27.33}$$

for any wide root. Nevertheless, they modify the quantization condition because of the formula

$$\chi_{II}(\theta) = \chi(\theta) + \chi(\theta-\mathrm{i}\pi) = -\mathrm{i}\ln\frac{\sinh\lambda(\mathrm{i}\pi-\theta)}{\sinh\lambda\theta}. \tag{27.34}$$

In general, complex roots cannot be created freely in the repulsive regime. They never contribute to the energy and merely describe the polarization degrees of freedom of soliton–anti-soliton multiparticle states. The phenomenon is quite different in the attractive regime.

27.3.2 Attractive regime

Now we analyze the domain $\lambda > 1$, where one expects the existence of $[\lambda]$ breathers.

First we consider the first breather B_1. In identifying a given configuration, we analyze its energy and the quantization condition for its momentum which is affected by the corresponding scattering matrix. We claim that the B_1 particle with momentum θ is described by a self-conjugate wide root $\theta^w = \theta + \mathrm{i}\frac{\pi}{2\lambda}(1+\lambda)$. It has the topological charge 0 and its energy is

$$\begin{aligned} E = -M\cosh_{II}(\theta^w) &= -M\cosh(\theta^w) + M\cosh\left(\theta^w - \mathrm{i}\frac{\pi}{\lambda}\right) \\ &= 2M\sin\left(\frac{\pi}{2\lambda}\right)\cosh\theta, \end{aligned} \tag{27.35}$$

as is expected since the mass $m_{B_1} = 2M\sin\frac{\pi}{2\lambda}$. To check the soliton-breather scattering matrix, we additionally introduce a hole with rapidity θ^h. The quantization condition at θ^h means that

$$(-1)^{\delta}\mathrm{e}^{\mathrm{i}Z(\theta^h)} = (-1)^{\delta+1}\mathrm{e}^{\mathrm{i}ML\sinh\theta^h}\mathrm{e}^{-\mathrm{i}\chi_{II}(\theta^h-\theta^w)} = 1. \tag{27.36}$$

Using the integral representation for χ or the bootstrap relations, it can be show that

$$\chi_{II}(\theta) = \chi(\theta) - \chi\left(\theta - \mathrm{i}\frac{\pi}{\lambda}\right) = \mathrm{i}\ln S^{+1}_{+1}(\theta) + \mathrm{i}\pi, \tag{27.37}$$

so the S^{+1}_{+1} scattering matrix is correctly reproduced. Similarly, putting two self-conjugate roots at $\theta^w_1 = \theta_1 + \mathrm{i}\frac{\pi}{2\lambda}(1+\lambda)$ and $\theta^w_2 = \theta_2 + \mathrm{i}\frac{\pi}{2\lambda}(1+\lambda)$ one can also check the $B_1 - B_1$ scattering matrix by analyzing $Z_{II}(\theta^w_1)$.

Higher odd breathers can be obtained by creating a sequence of wide roots $\theta^w_k = \theta_k + \mathrm{i}\frac{\pi}{2\lambda}(\lambda - 2n + 1)$ for $k = 1, \ldots, n$ such that the lowest root is still a wide root. Similar root arrays, in which the lowest root is the close one, describe polarization degrees of freedom of soliton–anti-soliton states and cannot be created freely. An analysis similar to the above one can confirm both the energy and scattering matrices of these states [58]. The even breathers can be represented by the sequence of wide roots $\theta^w_k = \theta_k + \mathrm{i}\frac{\pi}{2\lambda}(\lambda - 2n)$ for $k = 1, \ldots, n$.

27.4 Small volume expansion

The integral equation (27.17) describes the spectrum of the sine-Gordon theory for any volume L. For large volumes, it reproduces the results of the scattering theory. For small volumes, it has to be related to the $c = 1$ conformal field theory.

As was already shown in Sect. 23.3, the spectrum of the perturbed free massless boson can be written as

$$E_n(L) = \frac{2\pi}{L}\left[E_{|n\rangle} - \frac{1}{12} + \sum_k c_k(\mu)^k\left(\frac{2\pi}{L}\right)^{2k(h-1)}\right], \tag{27.38}$$

where $E_{|n\rangle}$ is the conformal energy of the unperturbed state $|n\rangle$ and h is the conformal weight of the perturbation in the sine-Gordon model. One possible check of the integral equation is to determine the spectrum numerically and to compare to the above perturbative formula. One can numerically check the first few c_k coefficients. Unfortunately, unlike to the previous Sect. 26, there is no method for an exact calculation of the coefficients c_k. What we can do exactly is

to calculate the conformal energy levels only. The energy and momentum eigenvalues can be expressed via L_0, $\bar{L}_0$ as

$$E(L) = \frac{2\pi}{L}\left(L_0 + \bar{L}_0 - \frac{1}{12}\right), \qquad P(L) = \frac{2\pi}{L}(L_0 - \bar{L}_0). \tag{27.39}$$

The Hilbert space is built up from the states

$$a_{-n_1}^{k_1}\cdots a_{-n_N}^{k_N}\bar{a}_{-\bar{n}_1}^{\bar{k}_1}\cdots\bar{a}_{-\bar{n}_{\bar{N}}}^{\bar{k}_{\bar{N}}}|n,m\rangle. \tag{27.40}$$

The energy and momentum eigenvalues can be calculated by using

$$L_0|n,m\rangle = \frac{1}{8\pi}\left(\frac{n}{r} + 2\pi m r\right)^2|n,m\rangle, \quad \bar{L}_0|n,m\rangle = \frac{1}{8\pi}\left(\frac{n}{r} - 2\pi m r\right)^2|n,m\rangle \tag{27.41}$$

and the commutation relations

$$[L_n, a_{-m}] = m a_{-m}, \qquad [\bar{L}_n, \bar{a}_{-m}] = m\bar{a}_{-m}. \tag{27.42}$$

Here, $r = b^{-1}$ is the compactifaction radius, related to λ via $\lambda = \frac{8\pi}{b^2} - 1$.

We can see from (27.39) that the small volume spectrum diverges as L^{-1}. A careful analysis of the integral equation shows that the roots either move to $\pm\infty$ as $\theta_j = \pm\ln\frac{2}{ML} + \cdots$, or stay around the origin. Actually the three region become infinitely far from each other in the limit $L \to 0$ and the integral equation can be substituted by three independent equations. To describe this regime, we define the left/right mover and central roots:

$$\theta_j = \pm\ln\left(\frac{2}{ML}\right) \pm \theta_j^{\pm}, \qquad \theta_j = \theta_j^0, \tag{27.43}$$

where both $\theta_j^{\pm}$ and θ_j^0 are of order $O(1)$. The Z function is chosen as

$$Z_{\pm}(\theta) = \lim_{L\to 0} Z\left(\theta \pm \ln\frac{2}{ML}\right), \qquad Z_0(\theta) = \lim_{L\to 0} Z(\theta). \tag{27.44}$$

Taking the $L \to 0$ limit in the integral equation, we get

$$\begin{aligned} Z_\alpha(\theta) &= \alpha e^{\alpha\theta} + g_\alpha(\theta|\{\theta_j^\alpha\}) \\ &\quad + 2\Im m\int_{-\infty}^{\infty} \mathrm{d}\theta'\, G(\theta - \theta' - \mathrm{i}\eta)\ln\left[1 + (-1)^\delta e^{\mathrm{i}Z_\alpha(\theta'+\mathrm{i}\eta)}\right], \end{aligned} \tag{27.45}$$

where $\alpha = \pm, 0$. In g_α we have the contribution of the roots θ_j^α and additionally: $\chi(\infty)(Q - Q^\pm)$ for $g_\pm$ and $\chi(\infty)(Q^- - Q^+)$ for g_0, where $Q^\pm$ are the topological charges of the left/right moving configurations. Then using the expressions for the energy and momentum, we have

$$\begin{aligned} \frac{L}{4\pi}\left[E(L) \pm P(L) + \frac{1}{12}\right] &= \frac{1}{2\pi}\left(\sum_{k=1}^{N_H^\pm} e^{\pm\theta_k^{h,\pm}} - \sum_{k=1}^{N_C^\pm} e^{\pm\theta_k^{c,\pm}} - \sum_{k=1}^{N_W^\pm} e_{II}^{\pm\theta_k^{w,\pm}}\right) \\ &\quad \mp \Im m\int_{-\infty}^{\infty} \mathrm{d}\theta\, e^{\pm\theta}\ln\left[1 + (-1)^\delta e^{\mathrm{i}Z_\pm(\theta+\mathrm{i}\eta)}\right]. \end{aligned} \tag{27.46}$$

Calculations lead to the conformal spectrum with

$$Q = m, \qquad n_{\pm} = \frac{\delta}{2} + k_{\pm} \mp \left(\frac{Q}{2} \mp Q^{\pm} \right), \tag{27.47}$$

where $k_{\pm}$ are integers such that $n_{+} = n_{-}$ [41]. The integer excitation numbers are related to the quantization numbers of left and right moving roots.

28 Two-dimensional Coulomb gas

28.1 Basic facts about 2D Coulomb gas

Let us consider an infinite d-dimensional space of points $\mathbf{r} \in \mathbb{R}^d$, having for simplicity vacuum dielectric constant $\epsilon = 1$. The Coulomb potential $\phi(\mathbf{r})$, induced by a unit charge at the origin $\mathbf{0}$, is the solution of the Poisson equation

$$\Delta\phi(\mathbf{r}) = -s_d\delta(\mathbf{r}), \tag{28.1}$$

where s_d is the surface area of the d-dimensional unit sphere; $s_2 = 2\pi$, $s_3 = 4\pi$, etc. According to this definition, the long-range tail of the Coulomb potential implies in the Fourier space the characteristic singular small-k behavior $\hat{\phi}(\mathbf{k}) = 1/k^2$ in any dimension. This maintains many generic properties (like screening and the related sum rules [59]) of "real" 3D Coulomb systems with $\phi(\mathbf{r}) = 1/r$, $\mathbf{r} \in \mathbb{R}^3$. In 2D of interest, we have

$$\phi(\mathbf{r}) = -\ln\left(\frac{r}{r_0}\right), \qquad \mathbf{r} \in \mathbb{R}^2. \tag{28.2}$$

The free length scale r_0, which fixes the zero point of the Coulomb potential, is set for simplicity to unity.

The symmetric Coulomb gas, sometimes referred to as the two-component plasma, consists of two species of pointlike particles, of opposite unit charges $q \in \{+1, -1\}$ (in our units, the elementary charge $e = 1$). The interaction energy E of a given set of particles $\{i\}$, with charges $\{q_i\}$ and at spatial positions $\{\mathbf{r}_i\}$, is given by

$$E(\{q_i, \mathbf{r}_i\}) = \sum_{(i<j)=1}^{N} v_{q_i q_j}(\mathbf{r}_i, \mathbf{r}_j), \qquad v_{qq'}(\mathbf{r}, \mathbf{r}') = qq'\phi(|\mathbf{r} - \mathbf{r}'|). \tag{28.3}$$

The particles are constrained to a domain Λ; since we are interested in bulk properties, we shall consider the thermodynamic limit $|\Lambda| \to \infty$; the infinite system is homogeneous and translationally invariant. The Coulomb gas is studied in thermodynamic equilibrium, via the grand canonical ensemble characterized by the (dimensionless) inverse temperature β and the couple of fugacities z_+ and z_- for particles with charge $q = +1$ and $q = -1$, respectively. Alternatively, chemical potentials μ_+ and μ_- can be defined by $z_\pm = \exp(\beta\mu_\pm)/\lambda^2$ where λ is the de Broglie thermal wavelength. The bulk Coulomb gas is neutral [60], and thus its bulk properties depend only on $\mu = (\mu_+ + \mu_-)/2$, i.e. on $\sqrt{z_+ z_-}$. It is therefore possible to set $z_+ = z_- = z$; at some places, in order to distinguish between the $+$ and $-$ charges, we shall keep the notation $z_\pm$. The grand partition function is defined by

$$\Xi(z_+, z_-) = \sum_{N_+=0}^{\infty} \sum_{N_-=0}^{\infty} \frac{z_+^{N_+}}{N_+!} \frac{z_-^{N_-}}{N_-!} Q(N_+, N_-), \tag{28.4}$$

where

$$Q(N_+, N_-) = \int_\Lambda \prod_{i=1}^{N} \mathrm{d}\mathbf{r}_i \, \exp\left[-\beta E(\{q_i, \mathbf{r}_i\})\right] \tag{28.5}$$

is the configuration integral of N_+ positive and N_- negative charges, and $N = N_+ + N_-$. Due to the neutrality of the bulk Coulomb gas, the sums in (28.4) over all possible values of N_+ and N_- may be restricted to neutral configurations $N_+ = N_- = N/2$ ($N = 0, 2, 4, \ldots$) only. For the 2D Coulomb potential (28.2) with $r_0 = 1$, the configuration integral reads

$$Q(N_+, N_-) = \int_\Lambda \prod_{i=1}^{N} \mathrm{d}^2 r_i \prod_{(i<j)=1}^{N} |\mathbf{r}_i - \mathbf{r}_j|^{\beta q_i q_j}. \tag{28.6}$$

The grand potential Ω is defined by

$$-\beta\Omega = \ln \Xi. \tag{28.7}$$

It is expected to be an extensive quantity, $\Omega \propto |\Lambda|$, in the thermodynamic limit. The specific grand potential ω is related to the bulk pressure P as follows

$$-\beta\omega = \lim_{|\Lambda|\to\infty} \frac{-\beta\Omega}{|\Lambda|} = \lim_{|\Lambda|\to\infty} \frac{\ln \Xi}{|\Lambda|} = \beta P. \tag{28.8}$$

For the considered case of pointlike particles, the singularity of the Coulomb potential of the Coulomb potential (28.2) at the origin $\mathbf{r} = \mathbf{0}$ can cause the thermodynamic collapse of positive-negative pairs of charges. The (short-distance, ultraviolet) stability against this collapse is associated with the 2D spatial integrability $\int \mathrm{d}r\, r$ of the corresponding Boltzmann factor $r^{-\beta}$ at short distances. We see that the stability regime corresponds to small enough inverse temperatures $0 \le \beta < 2$; in what follows, we shall restrict ourselves to this stability region. Going beyond $\beta = 2$, the introduction of a small hard core around each particle, keeping the $+/-$ pairs at some finite nonzero distance, is inevitable. In spite of the tendency to the creation of neutral pairs of $+/-$ charges, there still exist free charges (which are able to screen and so the system remains in its conducting phase) up to the Kosterlitz-Thouless transition of infinite order to the dielectric phase at point $\beta_{\mathrm{KT}} = 4$ [61].

In the complementary large-distance (infrared) region, the configuration integrals (28.6) diverge in the thermodynamic limit $|\Lambda| \to \infty$ provided that $\beta < 4$. To show this fact, we consider the configuration integral (28.6) with the imposed charge neutrality $N_+ = N_- = N/2$,

$$\begin{aligned} Q(N/2, N/2) \;=\; & \int_\Lambda \prod_{i=1}^{N/2} \mathrm{d}^2 p_i \prod_{i=1}^{N/2} \mathrm{d}^2 n_i \prod_{(i<j)=1}^{N/2} |\mathbf{p}_i - \mathbf{p}_j|^{\beta} \\ & \times \prod_{(i<j)=1}^{N/2} |\mathbf{n}_i - \mathbf{n}_j|^{\beta} \prod_{i,j=1}^{N/2} |\mathbf{p}_i - \mathbf{n}_j|^{-\beta}, \end{aligned} \tag{28.9}$$

where $\mathbf{p}$ ($\mathbf{n}$) denote the vector positions of positive (negative) charges. Since the thermodynamic limit should not depend on the shape of the domain Λ, we can choose the disc geometry of radius R. We rescale all $\mathbf{p}$ and $\mathbf{n}$ vectors in the integral (28.9) by R and obtain $Q(N/2, N/2) \propto R^{N(2-\beta/2)}$. If $\beta < 4$, $Q(N/2, N/2) \to \infty$ in the thermodynamic limit $R \to \infty$. This divergence will be eliminated within the so-called renormalized Mayer expansion, developed in the next subsection. For the time being, the infrared divergence causes that the grand potential Ω depends

on the fugacity z in a non-analytic way. Indeed, as $Q(N/2, N/2) \propto R^{N(2-\beta/2)}$ couples to z^N, Ω depends on z and R exclusively via the combination $zR^{2-\beta/2}$. But $\Omega \propto R^2$, so that

$$\beta P = -\beta\omega = f(\beta) z^{\frac{1}{1-\beta/4}} \tag{28.10}$$

with some as yet undetermined function of primary interest $f(\beta)$.

In order to introduce the one- and two-body densities, we need a functional generalization of the grand partition function to position-dependent fugacities $z_\pm \to z_\pm(\mathbf{r})$:

$$\Xi[z] = \sum_{N_+=0}^{\infty} \sum_{N_-=0}^{\infty} \frac{1}{N_+!} \frac{1}{N_-!} \int_\Lambda \prod_{i=1}^{N} [\mathrm{d}\mathbf{r}_i z_{q_i}(\mathbf{r_i})] \prod_{(i<j)=1}^{N} \mathrm{e}^{-\beta v_{q_i q_j}(\mathbf{r}_i, \mathbf{r}_j)}. \tag{28.11}$$

The density of particles with charge $q = \pm$, n_q, is defined by

$$n_q(\mathbf{r}) = \left\langle \sum_i \delta_{q,q_i} \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle = z_q(\mathbf{r}) \frac{1}{\Xi} \frac{\delta \Xi}{\delta z_q(\mathbf{r})} \bigg|_{\text{uniform}}. \tag{28.12}$$

Here, "uniform" means $z_+(\mathbf{r}) = z_-(\mathbf{r}) = z$ and the thermodynamic limit $|\Lambda| \to \infty$. Due to the space homogeneity, we have $n_+(\mathbf{r}) = n_-(\mathbf{r}) = n/2$, where the total particle density is given by

$$n = z \frac{\partial}{\partial z}(-\beta\omega) = f(\beta) \frac{1}{1-\beta/4} z^{\frac{1}{1-\beta/4}}. \tag{28.13}$$

The density-fugacity relation plays a fundamental role in the derivation of the thermodynamics. Comparing (28.13) with the relation (28.10), we obtain the exact equation of state

$$\beta P = \left(1 - \frac{\beta}{4}\right) n, \tag{28.14}$$

which is equivalent to the equation of state for an ideal fluid, with the particle density rescaled by the temperature-dependent factor $1 - \beta/4$.

At two-particle level, we introduce the translationally invariant two-body densities

$$\begin{aligned} n_{qq'}(\mathbf{r}, \mathbf{r}') &= \left\langle \sum_{i \neq j} \delta_{q,q_i} \delta(\mathbf{r} - \mathbf{r}_i) \delta_{q',q_j} \delta(\mathbf{r}' - \mathbf{r}_j) \right\rangle \\ &= z_q(\mathbf{r}) z_{q'}(\mathbf{r}') \frac{1}{\Xi} \frac{\delta^2 \Xi}{\delta z_q(\mathbf{r}) \delta z_{q'}(\mathbf{r}')} \bigg|_{\text{uniform}}. \end{aligned} \tag{28.15}$$

They describe the effect of statistical correlation between two particles, the one with charge q at spatial position $\mathbf{r}$ and the other with charge q' at $\mathbf{r}'$. For oppositely charged particles, the two-body densities possess an important property: Their behavior at short distance is dominated by the Boltzmann factor of the Coulomb potential [62],

$$n_{+-}(\mathbf{r}, \mathbf{r}') \sim z_+ z_- \frac{1}{|\mathbf{r} - \mathbf{r}'|^\beta}. \tag{28.16}$$

28.2 Renormalized Mayer expansion

For the 2D Coulomb gas, we can construct systematically the high-temperature expansion of the density-fugacity relationship (28.13) in powers of β. The method is based on a renormalization of the Mayer diagrammatic technique for general classical multi-component fluids; the charge q, which takes the $\pm$ values in the Coulomb gas, denotes internal degrees of freedom for particles. We first review the ordinary Mayer expansion and then explain its bond-series renormalization.

The above formulation with fugacities $\{z_q(\mathbf{r})\}$ as controlling variables and the logarithm of the grand partition function as the generator for one-particle densities (28.12) is the direct one. The transition to the inverse format, with densities $\{n_q(\mathbf{r})\}$ as controlling variables, is based on the Legendre transformation

$$-\beta F[n] = \ln \Xi - \int_\Lambda \mathrm{d}\mathbf{r} \sum_q n_q(\mathbf{r}) \ln z_q(\mathbf{r}), \tag{28.17}$$

which defines the Helmholtz free energy F as the explicit density functional. The subtraction of the one-particle part leads to the excess free energy F^{ex}, defined by

$$\Delta[n] \equiv -\beta F^{\mathrm{ex}}[n] = -\beta F[n] + \int_\Lambda \mathrm{d}\mathbf{r} \sum_q \left[n_q(\mathbf{r}) \ln n_q(\mathbf{r}) - n_q(\mathbf{r}) \right]. \tag{28.18}$$

It is easy to show that $\Delta[n]$ is the generator for the density-fugacity relationship in the following sense

$$\ln \left[\frac{n_q(\mathbf{r})}{z_q(\mathbf{r})} \right] = \frac{\delta \Delta[n]}{\delta n_q(\mathbf{r})}, \qquad q = \pm. \tag{28.19}$$

The ordinary Mayer diagrammatic technique (see e.g. the monograph [63]) is based on the introduction of the Mayer f-function, related to the pair interaction via

$$\exp\left[-\beta v_{qq'}(\mathbf{r}, \mathbf{r}')\right] = 1 + f_{qq'}(\mathbf{r}, \mathbf{r}'). \tag{28.20}$$

For "standard" interactions $v_{qq'}(\mathbf{r}, \mathbf{r}')$, which vanish for $|\mathbf{r} - \mathbf{r}'| \to \infty$, also $f_{qq'}(\mathbf{r}, \mathbf{r}')$ goes to 0 at asymptotically large distances. Inserting the decomposition (28.20) into the definition of the grand partition function (28.11), expanding in Mayer f-functions and using specific topological reduction rules for the obtained diagrams, in the density format, the Mayer diagrammatic representation of the generator $\Delta[n]$ reads

$$\begin{aligned} \Delta[n] \quad = \quad & \big\{ \text{all connected diagrams which consist of } N \geq 2 \text{ field } n_{q_i}(i)\text{-circles} \\ & \quad \text{and } f_{q_i q_j}(i,j)\text{-bonds, and are free of connecting circles.} \big\} \end{aligned} \tag{28.21}$$

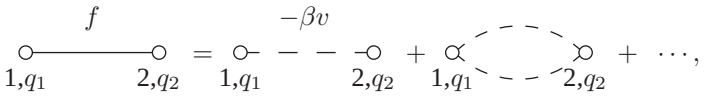
Here, the vector position $\mathbf{r}_i$ of a particle is denoted by i $(= 1, \ldots, N)$ and every field (black) circle i is integrated over spatial coordinate $\mathbf{r}_i$ and summed over q_i-states. A connecting circle is the one whose removal disconnects the diagram onto two or more independent parts.

The f-bonds are not integrable for the Coulomb gas. In this case, the renormalization of the Mayer expansion consists in two steps [64–66]:

- The expansion of each Mayer function in the inverse temperature,

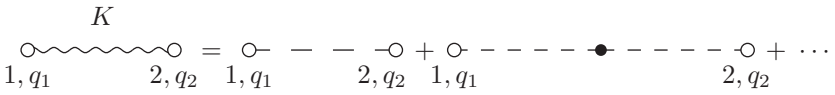
$$f_{q_1q_2}(1,2) = -\beta v_{q_1q_2}(1,2) + \frac{1}{2!}\left[-\beta v_{q_1q_2}(1,2)\right]^2 + \cdots \tag{28.22}$$

or, graphically,



where the factor 1/(number of interaction lines)! is automatically assumed.

- The consequent series elimination of two-coordinated field circles between every couple of three- or more-coordinated field circles; hereinafter, by coordination of a circle we mean its bond-coordination, i.e. the number of bonds meeting at this circle. The renormalized K-bonds are given by



or, algebraically,

$$\begin{aligned} K_{q_1q_2}(1,2) &= \left[-\beta v_{q_1q_2}(1,2)\right] \\ &\quad + \sum_{q_3}\int_\Lambda \mathrm{d}3\left[-\beta v_{q_1q_2}(1,3)\right] n_{q_3}(3) K_{q_3q_2}(3,2). \end{aligned} \tag{28.23}$$

The bond-renormalization transforms the ordinary Mayer diagrammatic expansion (28.21) into [66]

$$\Delta[n] = \quad + D_0[n] + \sum_{s=1}^{\infty} D_s[n], \tag{28.24}$$

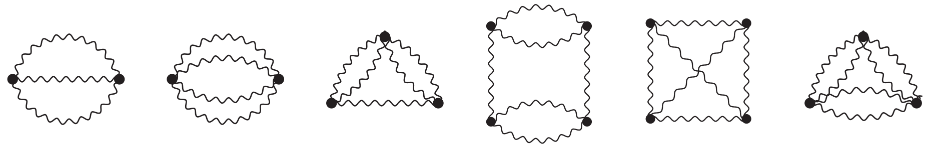
where

$$\begin{aligned} D_0[n] &= \quad + \quad + \quad + \cdots \\ &= \sum_{N=2}^{\infty}\frac{1}{2N}\sum_{q_1,\ldots,q_N}\int_\Lambda \prod_{i=1}^{N}\left[\mathrm{d}i\, n_{q_i}(i)\right]\left[-\beta v_{q_1q_2}(1,2)\right] \\ &\qquad \times\left[-\beta v_{q_2q_3}(2,3)\right]\cdots\left[-\beta v_{q_Nq_1}(N,1)\right] \end{aligned} \tag{28.25}$$

is the sum of all unrenormalized ring diagrams (which cannot undertake the renormalization procedure because of the absence of three- or more-coordinated field points) and

$$\sum_{s=1}^{\infty} D_s[n] = \Big\{\text{all connected diagrams which consist of } N \geq 2 \text{ field } n_{q_i}(i)\text{-circles of coordination} \geq 3 \text{ and multiple } K_{q_i q_j}(i,j)\text{-bonds, and are free of connecting circles}\Big\} \tag{28.26}$$

represents the set of all remaining completely renormalized graphs. By multiple K-bonds we mean the possibility of an arbitrary number of K-bonds between a couple of field circles, with the obvious topological factor $1/(\text{number of bonds})!$. The order of s-enumeration is irrelevant, let us say



D_1 D_2 D_3 D_4 D_5 D_6

etc.

In accordance with the relation (28.19), the density-fugacity relation is expressible in the renormalized format as follows

$$\ln\left[\frac{n_{q_1}(1)}{z_{q_1}(1)}\right] =$$ $$+\ d_0(1,q_1) + \sum_{s=1}^{\infty} d_s(1,q_1) \tag{28.27}$$

$1, q_1$

where the root (white) circle has the fixed spatial vector 1 and the particle state q_1, $d_0(1,q_1) = \delta D_0[n]/\delta n_{q_1}(1)$ can be readily obtained as the limit

$$d_0(1,q_1) = \frac{1}{2}\lim_{2\to 1}\left[K_{q_1 q_2}(1,2) + \beta v_{q_1 q_2}(1,2)\right]\Big|_{q_2=q_1} \tag{28.28}$$

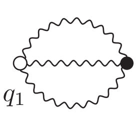
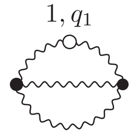
and

$$d_s(1,q_1) = \frac{\delta D_s[n]}{\delta n_{q_1}(1)} \qquad (s = 1,2,\ldots) \tag{28.29}$$

denotes the whole family of $(1,q_1)$-rooted diagrams generated from $D_s[n]$. To get the family, one has to take into account the functional dependence of the dressed K-bonds (28.23) on the species densities as well. Since it holds

$$\frac{\delta K_{q_1 q_2}(1,2)}{\delta n_{q_3}(3)} = K_{q_1 q_3}(1,3) K_{q_3 q_2}(3,2), \tag{28.30}$$

the root circle is generated, besides the field-circle positions, also on K-bonds, causing their "correct" $K-K$ division. For example, in the case of the generator D_1, we get

$d_1(1,q_1) =$  $+$  (28.31)

$1, q_1$

For the infinite 2D Coulomb gas with homogeneous species densities $n_q(\mathbf{r}) = n_q = n/2$ $(q = \pm)$, the renormalized K-bonds (28.23) take the form

$$K_{q_i q_j}(i,j) = q_i q_j K(i,j) \tag{28.32}$$

where $K(i,j)$ satisfies the integral equation

$$K(1,2) = [-\beta\phi(1,2)] + \int_\Lambda \mathrm{d}3\,[-\beta\phi(1,3)]\,nK(3,2). \tag{28.33}$$

Since $|\Lambda| \to \infty$, we have the translationally invariant $K(i,j) = K(|i-j|)$ and so this equation is explicitly solvable in the Fourier space. Recalling that the Fourier component $\hat{\phi}(k) = 1/k^2$, we arrive at

$$K(r) = -\beta \int \frac{\mathrm{d}^2 k}{2\pi} \frac{1}{k^2 + 2\pi\beta n} \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}) = -\beta K_0(r\sqrt{2\pi\beta n}), \tag{28.34}$$

where K_0 is the modified Bessel function of second kind.

The renormalized representation of the generator $\Delta(n)$, Eqs. (28.24)-(28.26), consists of three kinds of diagrams.

(i) The first term on the rhs of (28.24)

$$\frac{1}{2!} \sum_{q_1,q_2=\pm 1} \int_\Lambda \mathrm{d}1\mathrm{d}2\, q_1 n_{q_1}(1)\,[-\beta\phi(1,2)]\,q_2 n_{q_2}(2) \tag{28.35}$$

is equal to zero by the charge neutrality.

(ii) The second term (28.25) is expressible as

$$\begin{aligned} D_0(n) &= \sum_{N=2}^{\infty} \frac{n^N}{2N} \int_\Lambda \prod_{i=1}^{N} \mathrm{d}i\,[-\beta\phi(1,2)]\,[-\beta\phi(2,3)]\cdots[-\beta\phi(N,1)] \\ &= \frac{1}{2}\int_0^n \mathrm{d}n' \sum_{N=2}^{\infty} n'^{(N-1)} \int_\Lambda \prod_{i=1}^{N} \mathrm{d}i\,[-\beta\phi(1,2)]\,[-\beta\phi(2,3)]\cdots[-\beta\phi(N,1)]\,. \end{aligned} \tag{28.36}$$

With regard to the relation (28.33), the sum over N is nothing but $|\Lambda| \times \lim_{r\to 0}[K(r) + \beta\phi(r)]$ evaluated at $n = n'$. Taking into account the explicit form of K-bonds (28.34), we need the small-x expansion of $K_0(x)$ [67],

$$K_0(x) = -\ln\left(\frac{x}{2}\right) I_0(x) + \sum_{i=0}^{\infty} \frac{x^{2i}}{2^{2i}(i!)^2}\psi(i+1), \tag{28.37}$$

where

$$I_0(x) = \sum_{i=0}^{\infty} \frac{x^{2i}}{2^{2i}(i!)^2} \qquad \text{and} \qquad \psi(x) = \frac{d}{dx}\ln\Gamma(x)$$

is the psi function; in particular, $\psi(1) = -C$ with C being Euler's constant. We find that

$$\frac{D_0(n)}{|\Lambda|} = \frac{\beta}{4}(n\ln n - n) + \frac{\beta n}{2}\left[C + \frac{1}{2}\ln\left(\frac{\pi\beta}{2}\right)\right]. \tag{28.38}$$

(iii) Let the completely renormalized diagram D_s $(s = 1, 2, \ldots)$, belonging to the sum (28.26), be composed of N_s skeleton vertices $i = 1, \ldots, N_s$ of coordination $\nu_i \geq 3$ and L_s bonds $\alpha = 1, \ldots, L_s$; a given bond α is defined by an ordered pair of skeleton vertices $(\alpha_1 < \alpha_2)$ joint by this bond. The set of coordination numbers $\{\nu_i\}$ is constrained by $\sum_{i=1}^{N_s} \nu_i = 2L_s$ as every bond is shared by just two vertices. For $n_{q_i}(i) = n/2$, $D_s(n)$ can be formally expressed as

$$\begin{aligned} D_s(n) &= t_s \sum_{q_1,\ldots,q_{N_s}=\pm 1} \int_\Lambda \prod_{i=1}^{N_s} [\mathrm{d}i\, n_{q_i}(i) q_i^{\nu_i}] \prod_{\alpha=1}^{L_s} K(\alpha_1, \alpha_2) \\ &= t_s \left(\frac{n}{2}\right)^{N_s} \prod_{i=1}^{N_s} \left(\sum_{q_i=\pm 1} q_i^{\nu_i} \right) \int_\Lambda \prod_{i=1}^{N_s} \mathrm{d}i \prod_{\alpha=1}^{L_s} K(\alpha_1, \alpha_2), \end{aligned} \tag{28.39}$$

where t_s is the numerical topological factor. We see that $D_s(n) \neq 0$ if and only if the coordinations of all vertices $\{\nu_i\}$ are even numbers ≥ 4. Let us assume that this condition is fulfilled. In the limit $|\Lambda| \to \infty$, due to the invariance of the integrated product $\prod_{\alpha=1}^{L_s} K(\alpha_1, \alpha_2)$ with respect to a uniform shift in all integration variables $\{i\}$, one of these variables can be chosen as a reference put at the origin $\mathbf{0}$, with the simultaneous multiplication of the integral by the volume $|\Lambda|$,

$$D_s(n) = t_s n^{N_s} |\Lambda| \int \prod_{i=1}^{N_s} \mathrm{d}i\, \delta(j - \mathbf{0}) \prod_{\alpha=1}^{L_s} K(\alpha_1, \alpha_2). \tag{28.40}$$

Here, j is the vector position of an arbitrary one of the field circles $(1, \ldots, N_s)$. The scaling form of $K(\alpha_1, \alpha_2) = -\beta K_0(|\alpha_1 - \alpha_2|\sqrt{2\pi\beta n})$ permits us to perform the n- and β-classification of the integral in (28.40). Every dressed bond $K(\alpha_1, \alpha_2)$ brings the factor $-\beta$ and enforces the substitution $r' = r\sqrt{2\pi\beta n}$ which manifests itself as the factor $1/(2\pi\beta n)$ for each field-circle integration $\sim \int r\mathrm{d}r$. Since there are just $(N_s - 1)$ independent field-circle integrations in (28.40), we conclude that

$$\frac{D_s(n)}{|\Lambda|} = n\beta^{L_s - N_s + 1} d_s, \qquad d_s = \frac{D_s(n = 1, \beta = 1)}{|\Lambda|}. \tag{28.41}$$

The first nonzero diagram is D_2. It contributes to the β^3 order, with

$$d_2 = \frac{1}{2!4!} \int \frac{\mathrm{d}^2 r}{2\pi} K_0^4(\mathbf{r}) = \frac{1}{2!4!} \frac{7}{8} \zeta(3), \tag{28.42}$$

where ζ is the Riemann's zeta function. In the next β^4 order, only the diagram D_6 has all vertices even-coordinated and therefore survives, with

$$d_6 = \frac{1}{3!(2!)^3} \int \frac{\mathrm{d}^2 r_1}{2\pi} \int \frac{\mathrm{d}^2 r_2}{2\pi} K_0^2(\mathbf{r}_1) K_0^2(\mathbf{r}_2) K_0^2(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{3!(2!)^3} \frac{3}{16} \zeta(3), \tag{28.43}$$

etc. The above integrals of Bessel functions are evaluated by using the Fourier component of $K_0^2(\mathbf{r})$,

$$\hat{G}(\mathbf{k}) = \int \frac{\mathrm{d}^2 r}{2\pi} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} K_0^2(\mathbf{r}) = \int_0^\infty \mathrm{d}r\, r J_0(kr) K_0^2(r) = \frac{\ln\left[\frac{k}{2} + \sqrt{1 + \left(\frac{k}{2}\right)^2}\right]}{k\sqrt{1 + \left(\frac{k}{2}\right)^2}}, \tag{28.44}$$

where J_0 is the ordinary Bessel function. Simple algebra yields

$$\int \frac{\mathrm{d}^2 r}{2\pi} K_0^2(\mathbf{r}) K_0^2(\mathbf{r}) = \int_0^\infty \mathrm{d}k\, k\hat{G}^2(k) \tag{28.45}$$

and

$$\int \frac{\mathrm{d}^2 r_1}{2\pi} \frac{\mathrm{d}^2 r_2}{2\pi} K_0^2(\mathbf{r}_1) K_0^2(\mathbf{r}_2) K_0^2(\mathbf{r}_1 - \mathbf{r}_2) = \int_0^\infty \mathrm{d}k\, k\hat{G}^3(k). \tag{28.46}$$

The primitive functions of $k\hat{G}^2(k)$ and $k\hat{G}^3(k)$ are available explicitly [67].

The diagrammatic contributions in the above paragraphs (i)–(iii) can be summarized by the formula

$$\frac{\Delta(n)}{|\Lambda|} = \frac{\beta}{4}(n \ln n - n) + \frac{\beta n}{2}\left[C + \frac{1}{2}\ln\left(\frac{\pi\beta}{2}\right)\right] + n\sum_{s=1}^{\infty} d_s \beta^{L_s - N_s + 1}. \tag{28.47}$$

Here, $\{d_s\}$ are the numbers yielded by the topology of the renormalized diagrams $\{D_s\}$, nonzero only if the bond coordinations of all vertices are even numbers ≥ 4. The first few nonzero contributions read

$$\sum_{s=1}^{\infty} d_s \beta^{L_s - N_s + 1} = \frac{7}{6}\zeta(3)\left(\frac{\beta}{4}\right)^3 + \zeta(3)\left(\frac{\beta}{4}\right)^4 + O(\beta^5). \tag{28.48}$$

In order to evaluate $\ln(n_q/z_q)$ $(q = \pm)$ using the relation (28.19), we first recall the well-known equation

$$\frac{\partial \Delta(n)}{\partial n} = \sum_q \int \mathrm{d}\mathbf{r}\, \frac{\delta \Delta[n]}{\delta n_q(\mathbf{r})} \frac{\partial n_q(\mathbf{r})}{\partial n} \tag{28.49}$$

valid for an arbitrary functional $\Delta[n]$ with $n_q(\mathbf{r})$ substituted by some function of n. In the homogeneous case $n_+(\mathbf{r}) = n_-(\mathbf{r}) = n/2$, this relation takes the form

$$\frac{\partial \Delta(n)}{\partial n} = \frac{|\Lambda|}{2}\left(\frac{\delta \Delta[n]}{\delta n_+(\mathbf{r})}\bigg|_{\mathrm{uniform}} + \frac{\delta \Delta[n]}{\delta n_-(\mathbf{r})}\bigg|_{\mathrm{uniform}}\right), \tag{28.50}$$

where the $\mathbf{r}$-independence of the functional derivatives was assumed for an infinite system. For diagrams in $\Delta[n]$, the direct link between the $+$ and $-$ states of the root point is realized through the charge state transformation $\{q_i \to -q_i\}$ at all field vertices. The diagrams are invariant with respect to this transformation. Hence, taking into account (28.50), we have

$$\frac{\delta \Delta[n]}{\delta n_+(\mathbf{r})}\bigg|_{\mathrm{uniform}} = \frac{\delta \Delta[n]}{\delta n_-(\mathbf{r})}\bigg|_{\mathrm{uniform}} = \frac{\partial}{\partial n}\frac{\Delta(n)}{|\Lambda|}. \tag{28.51}$$

The consequent relations $\ln(n_+/z) = \ln(n_-/z) = \partial[\Delta(n)/|\Lambda|]/\partial n$, with $\Delta(n)/|\Lambda|$ given by (28.47), lead to the final result

$$\frac{n^{1-\beta/4}}{z} = 2\beta^{\beta/4} \exp\left\{\left[2C + \ln\left(\frac{\pi}{2}\right)\right]\frac{\beta}{4} + \sum_{s=1}^{\infty} d_s \beta^{L_s - N_s + 1}\right\}. \tag{28.52}$$

Taking into account (28.48), this represents the high-temperature (small β) expansion of the density-fugacity relation for the 2D Coulomb gas.

28.3 Mapping onto the sine-Gordon model

The 2D Coulomb gas is equivalent to the 2D Euclidean sine-Gordon model [68–70]. The mapping is accomplished via the grand partition function defined by (28.4) and (28.5). Introducing the microscopic charge density

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} q_i \delta(\mathbf{r} - \mathbf{r}_i), \tag{28.53}$$

the interaction energy (28.3) can be expressed as

$$E(\{q_i, \mathbf{r}_i\}) = \frac{1}{2} \int \mathrm{d}^2 r \int \mathrm{d}^2 r' \, \rho(\mathbf{r}) \phi(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') - \frac{1}{2} N \phi(0); \tag{28.54}$$

we forget for a while that the self-energy $\phi(0) = \lim_{r \to 0}(-\ln r)$ diverges. Let us consider the corresponding Boltzmann factor $\exp[-\beta E(\{q_i, \mathbf{r}_i\})]$ in the configuration integral (28.5). Since $-\Delta/(2\pi)$ is the inverse operator of the 2D Coulomb potential $\phi(\mathbf{r})$ [see Eq. (28.1) with $s_2 = 2\pi$], using the Hubbard-Stratonovich transformation we have

$$\exp\left[-\frac{\beta}{2} \int \mathrm{d}^2 r \int \mathrm{d}^2 r' \, \rho(\mathbf{r}) \phi(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}')\right] = \frac{\int \mathcal{D}\varphi \exp\left[\int \mathrm{d}^2 r \left(\frac{1}{2}\varphi \Delta \varphi + \mathrm{i} b \varphi \rho\right)\right]}{\int \mathcal{D}\varphi \exp\left(\int \mathrm{d}^2 r \frac{1}{2} \varphi \Delta \varphi\right)}, \tag{28.55}$$

where $b = \sqrt{2\pi\beta}$, $\varphi(\mathbf{r})$ is a real scalar field and $\int \mathcal{D}\varphi$ denotes the functional integration over this field. The term $\varphi \Delta \varphi$ can be rewritten as $-(\nabla\varphi)^2$ by using integration by parts, with a vanishing contribution from infinity. Inserting $\rho(\mathbf{r})$ from (28.53), the configuration integral is written as

$$Q(N_+, N_-) = \mathrm{e}^{\beta\phi(0)N/2} \left\langle \left(\int \mathrm{d}^2 r \, \mathrm{e}^{\mathrm{i} b \varphi(\mathbf{r})} \right)^{N_+} \left(\int \mathrm{d}^2 r \, \mathrm{e}^{-\mathrm{i} b \varphi(\mathbf{r})} \right)^{N_-} \right\rangle_{\text{free}}, \tag{28.56}$$

where $\langle \cdots \rangle_{\text{free}}$ means the average over the free-field action $S_{\text{free}} = \int \mathrm{d}^2 r \, (\nabla\varphi)^2/2$. The self-energy term renormalizes the fugacities,

$$\tilde{z}_\pm = \exp[\beta\phi(0)/2] z_\pm. \tag{28.57}$$

The grand partition function (28.4), after summing over N_+ and N_-, becomes the functional integral

$$\Xi(z_+, z_-) = \frac{\int \mathcal{D}\varphi \, \exp[-S(\tilde{z}_+, \tilde{z}_-)]}{\int \mathcal{D}\varphi \, \exp[-S(0,0)]} \tag{28.58}$$

with the action

$$S(\tilde{z}_+, \tilde{z}_-) = \int \mathrm{d}^2 r \, \left[\frac{1}{2}(\nabla\varphi)^2 - \tilde{z}_+ \mathrm{e}^{\mathrm{i} b \varphi} - \tilde{z}_- \mathrm{e}^{-\mathrm{i} b \varphi}\right]. \tag{28.59}$$

In the uniform case $z_+ = z_- = z$, we end up with the sine-Gordon representation

$$\Xi(z) = \frac{\int \mathcal{D}\varphi \, \exp[-S(\tilde{z})]}{\int \mathcal{D}\varphi \, \exp[-S(0)]}, \qquad S(\tilde{z}) = \int_\Lambda \mathrm{d}^2 r \, \left[\frac{1}{2}(\nabla\varphi)^2 - 2\tilde{z}\cos(b\varphi)\right], \tag{28.60}$$

where $\tilde{z} = \exp[\beta\phi(0)/2]z$ is the renormalized fugacity.

To obtain the sine-Gordon representation of the many-body densities, the generalization of the above formalism to position-dependent fugacities $z_\pm(\mathbf{r})$ is needed. The generalization is straightforward and results in the representation (28.58) with the action (28.59) in which the constant (renormalized) fugacities are substituted by the position-dependent ones, $\tilde{z}_\pm \to \tilde{z}_\pm(\mathbf{r})$. The one-body density (28.12) is obtained in the form

$$n_q(\mathbf{r}) = \frac{n}{2} = z_q(\mathbf{r})\frac{1}{\Xi}\frac{\delta\Xi}{\delta z_q(\mathbf{r})}\bigg|_{\text{uniform}} = \tilde{z}_q(\mathbf{r})\frac{1}{\Xi}\frac{\delta\Xi}{\delta \tilde{z}_q(\mathbf{r})}\bigg|_{\text{uniform}} = \tilde{z}\left\langle \mathrm{e}^{\mathrm{i}qb\varphi(\mathbf{r})}\right\rangle. \quad (28.61)$$

Here, the symbol $\langle\cdots\rangle$ denotes the averaging over the action (28.60), i.e.

$$\langle\cdots\rangle = \frac{1}{\int \mathcal{D}\varphi\, \exp[-S(\tilde{z})]}\int \mathcal{D}\varphi\, \exp[-S(\tilde{z})]\cdots. \quad (28.62)$$

For the two-body densities (28.15), we get

$$n_{qq'}(\mathbf{r},\mathbf{r}') = \tilde{z}_q(\mathbf{r})\tilde{z}_{q'}(\mathbf{r}')\frac{1}{\Xi}\frac{\delta^2\Xi}{\delta\tilde{z}_q(\mathbf{r})\delta\tilde{z}_{q'}(\mathbf{r}')}\bigg|_{\text{uniform}} = \tilde{z}^2\left\langle \mathrm{e}^{\mathrm{i}qb\varphi(\mathbf{r})}\mathrm{e}^{\mathrm{i}q'b\varphi(\mathbf{r}')}\right\rangle. \quad (28.63)$$

The crucial variable in the formalism is $\tilde{z}$, i.e. the fugacity renormalized by the diverging self-energy factor. In the sine-Gordon action $S(\tilde{z})$, it couples to the cos-field. To give $\tilde{z}$ a precise meaning, we have to fix the normalization of this cos-field. In the Coulomb format, the normalization is given by the short-distance behavior of the two-body density for oppositely charged particles (28.16). In view of (28.63), this short-distance asymptotic is equivalent to

$$\mathrm{e}^{\beta\phi(0)}\left\langle \mathrm{e}^{\mathrm{i}b\varphi(\mathbf{r})}\mathrm{e}^{-\mathrm{i}b\varphi(\mathbf{r}')}\right\rangle \sim \frac{1}{|\mathbf{r}-\mathbf{r}'|^\beta} \qquad \text{as } |\mathbf{r}-\mathbf{r}'| \to 0. \quad (28.64)$$

Under this so-called conformal normalization, which was usually omitted in statmech literature, the divergent self-energy factor disappears from statistical relations calculated within the sine-Gordon representation.

This fact can be easily verified in the high-temperature limit $\beta \to 0$, when, in the leading β order, $\cos(b\varphi) \sim 1 - (b\varphi)^2/2 = 1 - (\pi\beta)\varphi^2$. The sine-Gordon action $S(\tilde{z})$ becomes

$$S(\tilde{z}) \sim \int \mathrm{d}^2 r\left[\frac{1}{2}(\nabla\varphi)^2 + 2\pi\beta\tilde{z}\varphi^2\right] - 2\tilde{z}|\Lambda|. \quad (28.65)$$

Thus, φ has a Gaussian distribution. In terms of the Fourier component $\hat{\varphi}(\mathbf{k}) = \int \mathrm{d}^2 r\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\varphi(\mathbf{r})$, the φ-dependent part of the action takes the diagonal form

$$S(\tilde{z}) = \int \frac{\mathrm{d}^2 k}{(2\pi)^2}\left(\frac{k^2}{2} + 2\pi\beta\tilde{z}\right)|\hat{\varphi}(\mathbf{k})|^2. \quad (28.66)$$

Consequently,

$$\left\langle |\hat{\varphi}(\mathbf{k})|^2\right\rangle = \frac{1}{k^2 + 4\pi\beta\tilde{z}} \quad (28.67)$$

and

$$\langle\varphi(\mathbf{r})\varphi(\mathbf{r}')\rangle = \int \frac{\mathrm{d}^2 k}{(2\pi)^2}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\left\langle |\hat{\varphi}(\mathbf{k})|^2\right\rangle = \frac{1}{2\pi}K_0\left(\sqrt{4\pi\beta\tilde{z}}|\mathbf{r}-\mathbf{r}'|\right). \quad (28.68)$$

In the Gaussian approximation, it holds

$$\left\langle \mathrm{e}^{\mathrm{i}b[\varphi(\mathbf{r})-\varphi(\mathbf{r}')]} \right\rangle = \mathrm{e}^{-(b^2/2)\langle[\varphi(\mathbf{r})-\varphi(\mathbf{r}')]^2\rangle} = \mathrm{e}^{-\pi\beta\langle\varphi^2(\mathbf{r})\rangle}\mathrm{e}^{-\pi\beta\langle\varphi^2(\mathbf{r}')\rangle}\mathrm{e}^{2\pi\beta\langle\varphi(\mathbf{r})\varphi(\mathbf{r}')\rangle}. \tag{28.69}$$

In the large-distance limit $|\mathbf{r}-\mathbf{r}'| \to \infty$, $\langle \mathrm{e}^{\mathrm{i}b[\varphi(\mathbf{r})-\varphi(\mathbf{r}')]}\rangle$ decouples to $\langle \mathrm{e}^{\mathrm{i}b\varphi(\mathbf{r})}\rangle\langle \mathrm{e}^{-\mathrm{i}b\varphi(\mathbf{r}')}\rangle$ and, according to (28.68), $\langle\varphi(\mathbf{r})\varphi(\mathbf{r}')\rangle \to 0$. Thus we get

$$\mathrm{e}^{-\pi\beta\langle\varphi^2(\mathbf{r})\rangle} = \langle \mathrm{e}^{\pm\mathrm{i}b\varphi(\mathbf{r})}\rangle = \frac{n}{2\tilde{z}} \tag{28.70}$$

and the relation (28.69) reads

$$\left\langle \mathrm{e}^{\mathrm{i}b\varphi(\mathbf{r})}\mathrm{e}^{-\mathrm{i}b\varphi(\mathbf{r}')} \right\rangle = \left(\frac{n}{2\tilde{z}}\right)^2 \mathrm{e}^{2\pi\beta\langle\varphi(\mathbf{r})\varphi(\mathbf{r}')\rangle}. \tag{28.71}$$

In the short-distance limit $|\mathbf{r}-\mathbf{r}'| \to 0$, using the small-$x$ expansion of $K_0(x)$ (28.37) in (28.68), we have

$$\langle\varphi(\mathbf{r})\varphi(\mathbf{r}')\rangle \sim -\frac{1}{2\pi}\left[\ln\left(\sqrt{\pi\beta\tilde{z}}|\mathbf{r}-\mathbf{r}'|\right) + C\right]. \tag{28.72}$$

Combining this with the short-distance conformal normalization (28.64), the formula (28.71) leads to

$$\frac{n}{2z} = \exp\left\{\frac{\beta C}{2} + \frac{\beta}{4}\left[\ln(\pi\beta z) + \frac{\beta\phi(0)}{2}\right]\right\}. \tag{28.73}$$

But $\beta^2\phi(0) = 0$ at the order β; this term will be cancelled in the next β^2 order. We therefore conclude that

$$n = z^{1+\beta/4}2(\pi\beta)^{\beta/4}\exp\left(\frac{\beta C}{2}\right). \tag{28.74}$$

Since $1+\beta/4 \sim 1/(1-\beta/4)$ in the limit $\beta \to 0$, we recover the leading term of the density-fugacity relation (28.52) obtained by using the renormalized Mayer expansion.

28.4 Thermodynamics of the 2D Coulomb gas

The equivalence between the 2D Coulomb gas and the 2D Euclidean sine-Gordon theory is written in Eq. (28.60). For a large domain Λ, the sine-Gordon functional integral behaves as

$$\int \mathcal{D}\varphi\, \exp[-S(\tilde{z})] \sim \exp\left[-e_0(z)|\Lambda|\right], \tag{28.75}$$

where $e_0(z)$ is the specific ground state energy. This allows us to express the specific grand potential ω of the Coulomb gas (28.8) as follows

$$\beta\omega = e_0(z) - e_0(0), \tag{28.76}$$

where $e_0(0)$ is the specific ground-state energy of the free model.

From the exact TBA solution for the specific ground-state energy of the sine-Gordon model (26.62), we have

$$[e_0(z) - e_0(0)] = -\frac{M^2}{4} \tan\left(\frac{\pi\xi}{2}\right), \tag{28.77}$$

where ξ ($= 1/\lambda$ in the sine-Gordon model) is the temperature parameter given by

$$\xi = \frac{b^2}{8\pi - b^2} = \frac{\beta}{4-\beta}. \tag{28.78}$$

The fugacity z ($= \mu$ in the sine-Gordon model) is related to the soliton mass M by Eq. (26.69), written as

$$z = \frac{1}{\pi} \frac{\Gamma\left(\frac{\xi}{\xi+1}\right)}{\Gamma\left(\frac{1}{\xi+1}\right)} \left[M \frac{\sqrt{\pi}}{2} \frac{\Gamma\left(\frac{\xi+1}{2}\right)}{\Gamma\left(\frac{\xi}{2}\right)} \right]^{\frac{2}{\xi+1}}. \tag{28.79}$$

Finally, using the generating relation for the particle density (28.13), the explicit density-fugacity relationship reads

$$\frac{n^{1-\beta/4}}{z} = 2\left(\frac{\pi\beta}{8}\right)^{\beta/4} \frac{\Gamma\left(1-\frac{\beta}{4}\right)}{\Gamma\left(1+\frac{\beta}{4}\right)} \left[\frac{\tan\left(\frac{\pi\beta}{2(4-\beta)}\right)}{\frac{\pi\beta}{2(4-\beta)}} \frac{\Gamma^2\left(1+\frac{\beta}{2(4-\beta)}\right)}{\frac{1}{\pi}\Gamma^2\left(\frac{1}{2}+\frac{\beta}{2(4-\beta)}\right)} \right]^{1-\beta/4}. \tag{28.80}$$

The expansion of the rhs of this equation around the infinite temperature $\beta = 0$ up to the β^4 term is identical to the previous result (28.52) with the series (28.48). Near the collapse point $\beta = 2$ at fixed z, we get the expected divergence of the density:

$$n \sim \frac{4\pi z^2}{2-\beta}, \qquad \beta \to 2^-. \tag{28.81}$$

The same formula was derived by using a picture of the Coulomb gas near the collapse point as the system of independent neutral pairs of $+$ and $-$ charges [71].

To obtain the complete thermodynamics of the 2D Coulomb gas, we pass from the grand-canonical to canonical ensemble via the Legendre transformation

$$F = \Omega + \mu N, \tag{28.82}$$

where F is the free energy and $\mu = \beta^{-1} \ln z$. The knowledge of the density-fugacity relationship (28.80) allows us to obtain explicitly the free energy per particle $f = F/N$ as a function of the inverse temperature β and the particle density n. The derivatives of f with respect to β determine in the standard way the internal energy, the specific heat, etc. [72]. The extension of the exact thermodynamics of the 2D Coulomb gas beyond the collapse border $\beta = 2$ for particles with a small hard core (to prevent the collapse of opposite charges) was accomplished in Ref. [73].

We would like to emphasize that the 2D (symmetric) two-component Coulomb gas was the first classical fluid in dimension larger than one with completely known thermodynamics. Later [74], the thermodynamics of the Coulomb gas with the charge asymmetry $q_1 = +1$ and $q_2 = -1/2$ was solved by mapping the system onto the so-called complex Bullough-Dodd model [75]. This model is also integrable, for its TBA solution see Ref. [76].

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Zoltán Bajnok obtained his Master degree in physics from the Roland Eötvös University in 1992. In his thesis he analyzed conformal quantum field theories with extended symmetry. Afterwards he was awarded by a three year PhD fellowship of the Hungarian Academy of Sciences (HAS) and started to work on two-dimensional conformal field theories. By winning a visiting scholarship from the Széchenyi Research Foundation he worked in the Department of Applied Mathematics and Theoretical Physics in Cambridge between 1993-1994. This time he was invited to become a reviewer for Mathematical Reviews, and in 1994 he joined the American Mathematical Society. By defending his thesis in 1997 he became a Candidate in Physical Sciences. In 1997 he was awarded by a three year postdoctoral fellowship of the Hungarian National Science Foundation and started to work at the Theoretical Physics Department of Eötvös University. He gave yearly courses on theoretical physics for mathematicians and taught mathematical physics lectures for physicists. He started to train students who successfully participated in the national physics competitions. During the postdoctoral years he got involved in organizing and lecturing in summer schools. He became a member of the Hungarian Physical Society and the secretary of the Particle Physics Group. He also joined the particle physics committee of HAS. He got a position in the Theoretical Physics Research Group of HAS in 2000.

Being a physicist in heart, and also taking part in physics educational activities, he decided to work on more realistic models and their applications. He analyzed perturbed conformal field theories. His research was honored with a three year Bolyai Research Fellowship, awarded to young researchers of outstanding merit. Motivated by realistic systems with boundaries, he started to analyze integrable perturbations of boundary conformal field theories. He layed down the rigorous foundation of the bootstrap method and boundary quantum field theories. Based upon these results, he was invited to present his ideas at several conferences and, together with his Korean collaborators, was awarded by a 3-years exchange program between the Korean Science Foundation and HAS.

Later he started to apply the developed mathematical framework to physically relevant problems, such as to the boundary sine-Gordon theory, where he calculated exactly the spectrum of surface excitations. For these results he was awarded by the Theoretical Physical Novobátzky Prize of the Hungarian Physical Society in 2003 and was invited to give a plenary talk in MECO (Bratislava, 2004). This time he started to collaborate with Ladislav Šamaj in the field of Coulomb fluids.

In recent years he was applying two-dimensional integrable techniques to the description of planar AdS/CFT correspondence. Working on this topic he spent two months as a Marie Curie Research Fellow at the Jagellonian University of Cracow. In the year 2009 he completed his thesis on “Integrable models and the AdS/CFT correspondence” for which he was awarded by the title: Doctor of the Hungarian Academy of Sciences.

RNDr. Ladislav Šamaj, DrSc. graduated in theoretical condensed matter physics at the Comenius University in Bratislava (1983). The topic of his graduate thesis was "Recombination processes at grain boundaries of polycrystalline semiconductors". He received his PhD. degree at the Institute of Physics, Slovak Academy of Sciences, in 1988 with the thesis entitled "Analytic approaches to Ising lattice systems". In the same year, he got a permanent research position at the Institute of Physics, Slovak Academy of Sciences. In the years 1993-1996 and 1998, he was a researcher at the Courant Institute of Mathematical Sciences, New York University. He collaborated with Prof. Jerome K. Percus within an NSF grant in the field of exactly solvable density functionals for statistical lattice systems. At the same time, jointly with Profs. Jerome K. Percus and Joel L. Lebowitz from Rutgers University, he was the member of a NASA grant oriented to thermodynamics of lattice and continuum fluid systems. In 2000, he obtained a NATO fellowship by French NATO scientific committee to spend 9 months at Laboratoire de Physique Théorique, Université de Paris Sud in Orsay. He collaborated with Prof. Bernard Jancovici in the equilibrium statistical mechanics of exactly solvable Coulomb fluids. This collaboration lasts up to the present days, in the form of short-term visits and 2-3 months invited Professorships. The obtained results include the exact solution of the thermodynamics of the first fluid model in dimension larger than one, namely the two-dimensional Coulomb gas of pointlike ± 1 charges interacting via the logarithmic potential, the explanation of controversial high-temperature aspects of the electromagnetic Casimir effect, the consideration of retardation effects for charge correlation functions on the surface of a conductor, etc. During the years 2002-2008 he was in the editorial board of the Journal of Statistical Physics issued by Springer and since 2004 he is the member of the editorial board of the Journal of Statistical Mechanics (JSTAT) issued by IOP and SISSA. Dr. Šamaj was the principal investigator of three Slovak VEGA grants. Since 2005, he is the member of the Steering committee of the ESF project MISGAM (Methods of Integrable Systems, Geometry, Applied Mathematics). He published more than 70 scientific papers. For a series of papers entitled "Statistical mechanics of macroscopic systems: Exact results" he was awarded in 2007 by the Prize of Slovak Academy of Sciences for the basic research. Occasionally, he gives lectures about integrable many-body systems in quantum mechanics and statistical physics for PhD. students and researchers at the home Institute of Physics, Comenius University, Institute of Physics of Czech Academy of Sciences.