

SELF-CONSISTENT THEORY FOR THE Crossover FROM BCS
 SUPERCONDUCTIVITY TO BOSE-EINSTEIN CONDENSATION IN A
 FERMI LIQUID¹

R. Haussmann²

Sektion Physik der Ludwig-Maximilians-Universität München Theresienstrasse 37,
 D-80333 München, Germany

Received 13. April 1994, accepted 30 May 1994

A three-dimensional Fermi-liquid is considered with an instantaneous short-range interaction between the particles. The attractive interaction enables the formation of bound fermion pairs, which behave as bosons and condense to a superfluid at sufficiently low temperatures. Within the framework of many-body quantum-field theory we derive self-consistent equations for the fermion Greens function G and the vertex function Γ . While in mean-field approximation we obtain the BCS theory for weak coupling and the superfluid weakly interacting Bose gas for strong coupling, it turns out that in the intermediate region the self-consistency of the equations is essential for a proper treatment of the complicated interaction mechanisms of the fermions and the pairs. As a result we obtain a superfluid transition temperature T_c which increases monotonically with increasing attractive coupling strength. We find that the bound fermion pairs cause a power-law tail $\sim k^{-4}$ in the fermion occupation number $n(k)$ for large k and behave as short-living quasiparticles in the crossover region indicated by a complex effective mass $2m^*$ with a large imaginary part.

1. Introduction

Theories of superconductivity in strongly correlated electron systems beyond the Bardeen-Cooper-Schrieffer (BCS) theory have attracted a new interest since the discovery of high-temperature superconductivity in the copper oxides and more recently in the n-doped fullerenes. The main common feature of the high T_c superconductors is that $k_F\xi \sim 10$ -20 is comparatively small, which is due to the small electron density $n_F = k_F^3/3\pi^2$ of the doped systems and to the small coherence length ξ reflecting the small size of the Cooper pairs. In this paper we review the self-consistent theory of the crossover from BCS superconductivity in the weak-coupling regime $k_F\xi \gg 1$ to Bose-Einstein

¹Presented at MECO (Middle European CoOperation) 19, Smolenice, Slovakia, April 11-15, 1994
²e-mail address: Rudolf.Haussmann@stat.physik.uni-muenchen.de400.de

condensation of a fluid of tightly bound fermion pairs in the strong-coupling regime $k_F \xi \ll 1$. This theory has been developed by the author over the last two years [1, 2].

The simplest continuum system which exhibits the crossover scenario is a three-dimensional liquid of fermions of spin $1/2$ interacting instantaneously via an attractive potential. The interaction is assumed to be spin independent and of short range. The bound pairs that may form are assumed to have zero spin. The theory which is described in this paper treats the problem by the method of many-particle quantum-field theory with temperature dependent Greens functions [3, 4]. It is well known that superconductivity can not be described by standard perturbation theory. Much more the perturbation theory must be modified by resumming part of the Feynman diagrams. Superconductivity in a fermionic system is related to two different phenomena which must be treated properly in a successful theory. First, the attractive interaction between the fermions leads to the formation of bound pairs. Second, at low enough temperature the bound pairs condense into a *macroscopic* quantum-mechanically correlated state and form a superfluid. The first phenomenon is of *microscopic* nature and is properly treated by a resummation of topological classes of diagrams in the four-point vertex function Γ , which leads to the *Bethe-Salpeter equation*. The second phenomenon is taken into account by the partial summation of self-energy subgraphs which leads to the *Dyson equation*. This implies that in the remaining Feynman diagrams (skeleton diagrams) the fermion lines are identified as the exact fermion Greens function \mathcal{G} so that the resulting equations for \mathcal{G} and Γ are self-consistent. While \mathcal{G} describes the fermionic degrees of freedom, Γ is the effective scattering amplitude and plays the role of the boson propagator in the strong-coupling limit.

The crossover problem has been first investigated by Leggett [5] at zero temperature. Via a variational ansatz with a BCS trial wave function he derived two equations to determine the energy gap Δ and the chemical potential μ as functions of the coupling strength at $T = 0$ and for constant fermion density n_F . This variational ansatz has also been applied to the two-dimensional fermion system by Randeria, Duan, and Shieh [6]. Nozieres and Schmit-Rink [7] have extended the theory to finite temperatures by using the formalism with temperature dependent Greens functions and the ladder approximation, but *without* self consistency. While this theory was designed for $T \geq T_c$, they determined the critical temperature T_c in the whole crossover region from weak to strong coupling by the Thouless criterion [8]. A third approach is due to Drechsler and Zwerger [9]. Starting from a functional integral representation of the interacting fermion system Drechsler and Zwerger introduced the order parameter $\Delta(\mathbf{x}, \tau)$ via a Hubbard-Stratonovich transformation. Integrating out the fermion degrees of freedom and expanding in powers of $\Delta(\mathbf{x}, \tau)$ they obtained a Ginzburg-Landau theory. Though this theory was originally designed for a two-dimensional system [9], it has been extended recently to three dimensions [10]. Sá de Melo, Randeria, and Engelbrecht [11] have proposed a time dependent Ginzburg-Landau theory, and in close analogy to [7] they determined the superfluid transition temperature T_c which exhibits a small maximum in the crossover region.

All these previous theories are based on an approximation scheme which is equivalent to a mean-field approximation and which uses *free* fermion Greens functions to

take the fermionic degrees of freedom into account, while the bosonic properties lead to the superfluid transition. In the two limiting cases of weak and strong coupling this approximation leads to correct results. However, in the crossover region this approximation is invalid because the fermionic quasiparticles are rather short living and far from being free particles. Furthermore in this approximation in the strong-coupling regime the interaction between the noncondensed bosons is missed. Thus it turns out that self-consistency is essential in the crossover region to treat the nontrivial spectra and the complicated interaction mechanisms of the short-living fermionic and bosonic quasiparticles correctly.

In section 2 we derive two sets of self-consistent equations for the fermion Greens function \mathcal{G} and the vertex function Γ . We assume a *dilute* Fermi liquid with short-range interaction between the particles where the fermions are moving sufficiently slowly (at low temperature). Thus we can use the ladder approximation for the vertex function, and the interaction is taken into account satisfactorily by the inverse s -wave scattering length a_F^{-1} of the fermions. In section 3 we consider the mean-field approximation which turns out to be good in the two limiting cases of weak and strong interaction. While for weak coupling the BCS theory is recovered, in the strong-coupling limit the theory of the superfluid weakly interacting Bose gas is obtained where the bosons are identified as fermion pairs. In this way it is shown that the self-consistent theory describes the two standard possibilities of superfluidity as limiting cases within a unique framework. We have solved the self-consistent equations numerically for different coupling strengths at the superfluid transition $T = T_c$. In section 4 we present our results for T_c and μ_c as functions of the coupling strength. It turns out that T_c is a monotonic function for increasing coupling strength in contrast to the results of the previous theories which neglect self consistency. Furthermore we determine the effective mass $2m^*$ of the bound fermion pairs and the fermion occupation number $n(k)$. Due to a damping mechanism related to the pair breaking and recombination the effective mass $2m^*$ becomes complex in the weak-coupling and the intermediate regime. The bound fermion pairs cause power law tails $\sim k^{-4}$ in the fermion occupation number $n(k)$ for large momenta k .

2. The self-consistent equations for superfluid dilute Fermi liquids

The fermionic degrees of freedom of a superfluid Fermi liquid are described by the normal Greens function

$$\langle T[\psi_{\sigma_1}(\mathbf{x}_1, \tau_1)\psi_{\sigma_2}^+(\mathbf{x}_2, \tau_2)] \rangle = \delta_{\sigma_1\sigma_2} \cdot \mathcal{G}(\mathbf{x}_1 - \mathbf{x}_2, \tau_1 - \tau_2) \quad (2.1)$$

and the anomalous Greens function

$$\langle T[\psi_{\sigma_1}(\mathbf{x}_1, \tau_1)\psi_{\sigma_2}(\mathbf{x}_2, \tau_2)] \rangle = \epsilon_{\sigma_1\sigma_2} \cdot \mathcal{F}(\mathbf{x}_1 - \mathbf{x}_2, \tau_1 - \tau_2) \quad (2.2)$$

Since we assume that the interaction between the fermions is spin independent and the pairs that may form have zero spin, the normal Greens function is diagonal and the anomalous Greens function is antisymmetric in the spin indices. This fact is represented by the Kronecker symbol $\delta_{\sigma_1\sigma_2}$ in (2.1) and by the two-dimensional Levi-Civita tensor

$\epsilon_{\alpha_1\alpha_2}$ in (2.2). It turns out [1] that in the field-theoretic considerations the spin indices need not be treated explicitly. The spin-degrees of freedom are sufficiently taken into account by a factor 2 for each closed fermion line in a Feynman diagram. Thus the fermion (Greens functions (2.1) and (2.2) can be taken together into a 2×2 matrix Greens function

$$(\mathcal{G}_{\alpha_1\alpha_2}(\mathbf{x}, \tau)) = \begin{pmatrix} \mathcal{G}(\mathbf{x}, \tau) & \mathcal{F}(\mathbf{x}, \tau) \\ \mathcal{F}^*(-\mathbf{x}, \tau) & -\mathcal{G}(-\mathbf{x}, -\tau) \end{pmatrix} \quad (2.3)$$

We define the Fourier transformed Greens function $\mathcal{G}_{\alpha_1\alpha_2}(\mathbf{k}, \omega_n)$ by

$$\mathcal{G}_{\alpha_1\alpha_2}(\mathbf{x}, \tau) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\beta} \sum_{\omega_n} \exp[i(\mathbf{k}\mathbf{x} - \omega_n\tau)] \cdot \mathcal{G}_{\alpha_1\alpha_2}(\mathbf{k}, \omega_n) \quad (2.4)$$

where \mathbf{k} corresponds to the momentum of the fermions and $\omega_n = \pi(2n+1)k_B T/\hbar$ is the fermionic Matsubara frequency. Now, applying the formalism of many-particle quantum-field theory the fermion Greens function $\mathcal{G}_{\alpha_1\alpha_2}(\mathbf{k}, \omega_n)$ can be expressed in terms of the self energy $\Sigma_{\alpha_1\alpha_2}(\mathbf{k}, \omega_n)$ by

$$\mathcal{G}_{\alpha_1\alpha_2}^{-1}(\mathbf{k}, \omega_n) = -i\hbar\omega_n\delta_{\alpha_1\alpha_2} + \epsilon_{\mathbf{k}}\gamma_{\alpha_1\alpha_2} - \Sigma_{\alpha_1\alpha_2}(\mathbf{k}, \omega_n) \quad (2.5)$$

where $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m - \mu$ is the energy spectrum of the free fermions and $(\gamma_{\alpha_1\alpha_2})$ is a diagonal matrix similar to $(\delta_{\alpha_1\alpha_2})$ but with the diagonal elements 1 and -1 . In perturbation theory the self energy Σ is given by all one-particle irreducible Feynman graphs with two amputated external lines. However, since superconductivity is not accessible perturbatively, we must sum up the diagrams partially. Dyson's equation implies that the self energy Σ can be expressed in terms of the exact matrix-Greens function \mathcal{G} and the exact four-point vertex function Γ . This is shown in Fig. 1 in terms of Feynman diagrams where the indices and arguments are suppressed for simplicity. In Fig. 1a one clearly sees that the higher order diagrams of the self energy Σ are represented by the vertex function Γ which is given by the infinite perturbation series of Fig. 1b. The interaction between the fermions is represented by the elementary vertex shown in Fig. 1d. In all the diagrams of Figs. 1a and 1b we assume that already a partial summation over all self-energy subgraphs is performed. Hence the full lines in the diagrams are identified as the exact fermion Greens function \mathcal{G} (Fig. 1c). An orientation of the propagator lines is not necessary because the matrix Greens function (2.3) includes both directions. Thus one clearly sees that Eq. (2.5) together with the Dyson equation in Fig. 1a and the vertex function in Fig. 1b form a closed set of self-consistent equations for the fermion Greens function \mathcal{G} and the vertex function Γ . Since \mathcal{G} and Γ are matrices which have nonzero nondiagonal elements below T_c , the partial summation over all self-energy subgraphs leading to the self-consistent equations is the essential tool for describing the superfluid state.

A second partial summation of the diagrams of the vertex function in Fig. 1b is necessary to account for the formation of fermion pairs. To do this we divide the infinite set of diagrams into different topological classes as shown in Fig. 2a. The shaded circles



Fig. 1. (a) Dyson's equation for the self energy Σ ; (b) the infinite perturbation series for the exact vertex function Γ ; (c) full lines in the diagrams correspond to the exact fermion Greens function \mathcal{G} ; (d) the elementary vertex V .

on the right-hand side respectively represent the irreducible vertex function which is a partial sum of an infinite number of subgraphs. The irreducible vertex function is defined in such a way that the diagrams in Fig. 2a do not fall into two pieces if any two fermion lines *inside* one of the shaded circles are cutted. The infinite series of topological classes on the right hand side of Fig. 2a can be summed up as the geometric series. The result is the Bethe-Salpeter equation for the vertex function Γ which is shown in Fig. 2b. This equation is well suited to describe the formation of bound fermions pairs.

Until now we have described the exact theory. The self-consistent equations are given by (2.5), Fig. 1a, and Fig. 2b. The nontrivial infinite perturbation series is contained in the irreducible vertex function, which may be interpreted as an effective interaction of the fermions. Now, within this infinite perturbation series the approximation has to be performed. In the lowest order approximation we only take the leading contribution into account and thus replace the irreducible vertex function (shaded circle) by the bare interaction potential (elementary vertex, Fig. 1d). In this way we obtain the vertex function in *ladder approximation* [3,4] which is known to be a good approximation for a dilute system of fermions with a short-range interaction. Furthermore we assume that the fermions are moving slowly (at low temperature) and may form pairs with spin zero. Thus the details of the interaction potential $V(r)$ are not needed. According to Galtsov [12] and to Gorkov and Melik-Barkhadarov [13] the interaction potential can be replaced by the scattering amplitude T (the so-called T matrix) so that finally the interaction is satisfactorily taken into account by the s-wave scattering length a_f of the fermions. Neglecting of the particle-hole scattering reduces the vertex function to a 2×2 matrix $\Gamma_{\alpha_1\alpha_2}(\mathbf{K}, \Omega_n)$ which depends on the momentum $\hbar\mathbf{K}$ of the mass center of the two incoming or outgoing fermions and on the related bosonic Matsubara frequency $\Omega_n = 2\pi n k_B T/\hbar$. Since the s-wave scattering is isotropic, the vertex function does not

depend on the relative momenta of the incoming and the outgoing particles. This leads to a considerable simplification because the Bethe-Salpeter equation becomes a simple algebraic equation which is solved easily by a matrix inversion.

More details of the approximations are found in Ref. 1. Now we present the resulting self-consistent equations. In the ladder approximation the Bethe-Salpeter equation (Fig. 2b) implies that the two terms of the self energy in Fig. 1a can be combined into a single one-loop diagram with an exact Γ (solid circle) as vertex. Thus in real space the Dyson equation (Fig. 1a) can be written simply as

$$\Sigma_{\alpha_1\alpha_2}(\mathbf{x}, \tau) = G_{\alpha_2\alpha_1}(-\mathbf{x}, -\tau) \cdot \Gamma_{\alpha_1\alpha_2}(\mathbf{x}, \tau) \quad (2.6)$$

The Bethe-Salpeter equation reduces to an explicit expression for the inverse vertex function

$$\Gamma_{\alpha_1\alpha_2}^{-1}(\mathbf{K}, \Omega_n) = \frac{m}{4\pi\hbar^2} [a_F^{-1} \cdot \delta_{\alpha_1\alpha_2} + M_{\alpha_1\alpha_2}(\mathbf{K}, \Omega_n)] \quad (2.7)$$

where in real space the kernel is

$$M_{\alpha_1\alpha_2}(\mathbf{x}, \tau) = \frac{4\pi\hbar^2}{m} \left[G_{\alpha_1\alpha_2}(\mathbf{x}, \tau) \right]^2 - c \cdot \delta_{\alpha_1\alpha_2} \delta(\mathbf{x}) \cdot \hbar \sum_n \delta(\tau - n\hbar) \beta \quad (2.8)$$

Thereby c is an infinite renormalization constant which is defined such that $M_{\alpha_1\alpha_2}(\mathbf{x}, \tau)$ is obtained in *dimensional regularization* (see Ref. 1). For dimensions $2 < d < 4$ this renormalization is needed in the procedure of replacing the interaction potential by the scattering amplitude. The self-consistent equations (2.5)-(2.8) represent the simplest model for a continuous interacting Fermi system which exhibits the crossover scenario from BCS superconductivity to Bose-Einstein condensation of tightly bound pairs, where the interaction is parametrized by the inverse s -wave scattering length a_F^{-1} . It turns out that the conservation of the particle density is not invalidated by the approximations. The interaction is weak for $a_F^{-1} \ll -k_F$ and strong for $a_F^{-1} \gg +k_F$, where $k_F = (3\pi^2 n_F)^{1/3}$ is the Fermi wave number. The threshold where in scattering theory a virtual state turns over into a bound state is located at $a_F^{-1} = 0$. The crossover scenario happens in the interval $-k_F \lesssim a_F^{-1} \lesssim +k_F$.

3. Mean-field approximation and the limiting cases of weak and strong interaction

Since the vertex function $\Gamma_{\alpha_1\alpha_2}(\mathbf{K}, \Omega_n)$ describes the bosonic degrees of freedom of the system and in the strong-coupling limit it becomes even proportional to the boson Greens function of the pairs, it is natural to define the order parameter Δ of the superfluid transition by

$$\lim_{\mathbf{x} \rightarrow \infty} \Gamma_{\alpha_1\alpha_2}(\mathbf{x}, \tau) = \Gamma_{\alpha_1\alpha_2}^0 \quad (3.1)$$

with

$$\Gamma_{\alpha_1\alpha_2}^0 = - \begin{pmatrix} |\Delta|^2 & \Delta^2 \\ (\Delta^*)^2 & |\Delta|^2 \end{pmatrix} \quad (3.2)$$

While the self-consistent equations can not be solved analytically in general, a mean-field approximation can be constructed in the following way. Inserting approximately $\Gamma_{\alpha_1\alpha_2}^0$ for the vertex function into (2.6) then (2.5) and (2.6) can be solved *exactly* for the matrix Greens function. As a result we obtain the mean-field normal and anomalous Greens functions

$$G(\mathbf{k}, \omega_n) = u_{\mathbf{k}}^2 \frac{1}{-i\hbar\omega_n + E_{\mathbf{k}}} - v_{\mathbf{k}}^2 \frac{1}{i\hbar\omega_n + E_{\mathbf{k}}} \quad (3.3)$$

$$\mathcal{F}(\mathbf{k}, \omega_n) = -\frac{\Delta}{|\Delta|} u_{\mathbf{k}} v_{\mathbf{k}} \cdot \left[\frac{1}{-i\hbar\omega_n + E_{\mathbf{k}}} + \frac{1}{i\hbar\omega_n + E_{\mathbf{k}}} \right] \quad (3.4)$$

respectively, where $E_{\mathbf{k}} = [\epsilon_{\mathbf{k}}^2 + |\Delta|^2]^{1/2}$ is the energy spectrum of the fermionic quasiparticles and $u_{\mathbf{k}} = [(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})/2E_{\mathbf{k}}]^{1/2}$ and $v_{\mathbf{k}} = [(E_{\mathbf{k}} - \epsilon_{\mathbf{k}})/2E_{\mathbf{k}}]^{1/2}$ are the coefficients of a canonical transformation which satisfy the relations $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$, $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = \epsilon_{\mathbf{k}}/E_{\mathbf{k}}$, and $u_{\mathbf{k}} v_{\mathbf{k}} = |\Delta|/2E_{\mathbf{k}}$. Obviously, Eqs. (3.3) and (3.4) represent the well known normal and anomalous Greens functions of the BCS theory which, however, in this case are defined for arbitrary coupling strengths. Inserting these Greens functions into (2.8) and calculating the vertex function by (2.7), we obtain from (3.1) and (3.2) the self-consistency condition which in the thermodynamic limit leads to the well known BCS gap equation to determine the order parameter (energy gap) Δ . Thus it turns out that in the weak-coupling limit the results of the BCS theory can be recovered. Especially for the superfluid transition temperature we obtain the well known result [5]

$$T_c = (e^{\gamma_E}/\pi) \cdot (8/e^2) \cdot (\epsilon_F/k_B) \cdot \exp(\pi/2k_F a_F) \quad (3.5)$$

for $a_F^{-1} \ll -k_F$ (where $\gamma_E = 0.5772$ is the Euler number).

In the strong-coupling limit $a_F^{-1} \rightarrow +\infty$ the inverse matrix vertex function (2.7) can be evaluated explicitly. We obtain [1]

$$(\Gamma_{\alpha_1\alpha_2}^{-1}(\mathbf{K}, \Omega_n))^{-1} = -\frac{1}{8\pi c_b^2 a_F^3} \begin{pmatrix} -i\hbar\Omega_n + \frac{\hbar^2 \mathbf{K}^2}{4m} + \frac{|\Delta|^2}{2c_b} & -\frac{\Delta^2}{2c_b} \\ -\frac{(\Delta^*)^2}{2c_b} & i\hbar\Omega_n + \frac{\hbar^2 \mathbf{K}^2}{4m} + \frac{|\Delta|^2}{2c_b} \end{pmatrix} \quad (3.6)$$

for $a_F^{-1} \gg +k_F$ where $c_b = \hbar^2/m a_F^2$ is the binding energy of the pairs. In this formula one clearly sees that the matrix is an inverse matrix Greens function of a bosonic system. Thus, in the strong-coupling limit the vertex function Γ can be identified as $-[8\pi c_b^2 a_F^3]$ times the boson Greens function of the pairs. Furthermore, one can show that the main results of the theory of the superfluid weakly interacting Bose gas can be derived. Especially from the non diagonal elements in (3.6) we read off a repulsive interaction between the bosons which is due to the Pauli exclusion principle. We find a boson scattering length which is twice the fermion scattering length, $a_B = 2a_F$ [1]. This repulsive interaction leads to a slight depression of the transition temperature T_c compared to the temperature of the Bose-Einstein condensation. Thus we obtain

$$T_c = \frac{2\pi\hbar^2}{2mk_B} \left(\frac{n_F/2}{c(3/2)} \right)^{2/3} \cdot \left[1 - \frac{1}{3\pi} (k_F a_F)^3 + \dots \right] \quad (3.7)$$

for strong couplings $a_F^{-1} \gg +k_F$, where the second term in the square bracket goes beyond mean-field theory.

4. Numerical results

The mean-field approximation is good in the two limiting cases but invalid in the crossover region, because the fermionic quasiparticles have a short lifetime in the intermediate region while the mean-field Greens functions (3.3) and (3.4) treat the quasiparticles as stable. Thus for intermediate coupling strengths $-k_F \lesssim a_F^{-1} \lesssim +k_F$ the self-consistency is essential and the equations (2.5)-(2.8) must be solved numerically. This can be done by the following iteration procedure. We start by inserting the free (mean-field) fermion Greens function G_0 into (2.8) and (2.6) and then determine Γ and G_1 in first order by (2.7) and (2.5), respectively. The next iteration step is done by inserting the first order G into (2.8) and (2.6) again. The iteration procedure is repeated until convergence is achieved. It turns out that in practice 13 iterations are sufficient. While in (2.5) and (2.7) the functions are represented in Fourier space, in (2.6) and (2.8) the functions are represented in real space. Thus we need a numerical Fourier transformation for performing the iteration procedure. Since the functions G and Γ have rather nontrivial singularities, we have to transform functions which vary characteristically on a logarithmic scale over 6 to 10 decades. Since in this case the standard fast Fourier transformation [14] can not be used (because it assumes a constant stepwidth) we have invented a special slow Fourier transformation which is described in the appendix of Ref. 2. We discretise the functions over 6 to 10 decades with only 100 points in each dimension, interpolate the functions in between with cubic spline polynomials, and evaluate the Fourier integrals exactly. Since the physical system is spherically symmetric and the Fourier transformations can be reduced to two dimensions, the numerical effort is comparatively moderate so that a high-performance computer is not necessary.

The results of the numerical calculations are the fermion Greens function $G(\mathbf{k}, \omega_n)$ and the vertex function $\Gamma(\mathbf{K}, \Omega_n)$. From these functions several physical quantities can be read off. Since we have performed the numerical calculations for $T = T_c$, the anomalous Greens and vertex functions are zero. The superfluid transition is determined by the Thouless criterion $[\Gamma(\mathbf{K} = 0, \Omega_n = 0)]^{-1} = 0$ [8]. Thus, if the fermion density n_F is fixed, we obtain the transition temperature T_c and the related chemical potential μ_c as functions of the interaction strength a_F^{-1} . It turns out that the self-consistent equations (2.5)-(2.8) are scale invariant. Thus it is convenient to introduce dimensionless quantities which are scaled with the Fermi wave number $k_F = (3\pi^2 n_F)^{1/3}$. In this way n_F is automatically kept fixed. In Fig. 3 we present our numerical result for T_c versus the dimensionless coupling strength $v = 1/k_F a_F$ as full line. One clearly sees that $T_c(v)$ is a continuous function which increases monotonically with increasing v . The full line interpolates between the BCS result (3.5) for weak coupling (left-hand dashed line) and the asymptotic formula (3.7) for strong coupling (right-hand dashed line). For comparison we have determined $T_c(v)$ also from the first order vertex function Γ (first iteration). The result is shown as dotted line in Fig. 3. This approximation is equivalent to the theory of Nozières and Schmitt-Rink [7] and to the mean-field theories [9, 11]. The main feature of these previous theories is the maximum of $T_c(v)$ in the crossover

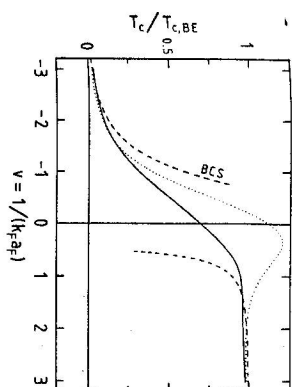


Fig. 3. The superfluid transition temperature $T_c(v)$ as a function of the dimensionless coupling strength $v = 1/k_F a_F$ for constant fermion density n_F . The full line represents the numerical result of our self-consistent theory. The dotted line is obtained by neglecting self-consistency and is similar to the results of the previous theories [7, 11]. The left-hand dashed line corresponds to the BCS theory, (3.5). The right-hand dashed line corresponds to our first order asymptotic formula (3.7) including the interaction between the fermion pairs.

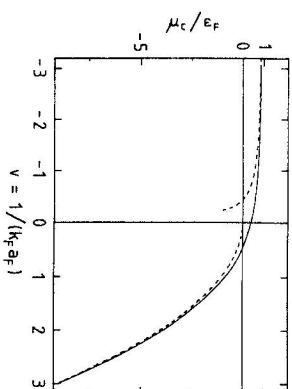


Fig. 4. The chemical potential μ_c at the superfluid transition as a function of the dimensionless coupling strength $v = 1/k_F a_F$. The full line represents our numerical result. The asymptotic result for the weakly interacting Fermi gas is shown as left-hand dashed line. The right-hand dashed line corresponds to the binding energy of the fermion pairs divided by 2.

region, which is clearly seen for the dotted curve in Fig. 3 as a considerable effect. While Nozières and Schmitt-Rink have pointed out that this maximum should be unphysical and presumably due to the approximations, we have found that the maximum is caused by the deficiency of the interaction between the (noncondensed) bosons in the mean-field approximation (first iteration). Going one order beyond this approximation, in the strong-coupling limit we have found a repulsive interaction between the bosons with scattering length $a_B = 2a_F$ which causes the second term in the asymptotic formula of T_c (3.7). Because of this term $T_c(v)$ is a monotonically increasing function at least for strong couplings (right-hand dashed line in Fig. 3) in contrast to the dotted line.

In Fig. 4 the chemical potential μ_c at the superfluid transition is shown in units of the Fermi energy $\epsilon_F = \hbar^2 k_F^2 / 2m$ as a function of the dimensionless coupling strength $v = 1/k_F a_F$. The full line represents our numerical result and interpolates between the weakly interacting Fermi gas (left-hand dashed line, $\mu_c \rightarrow \epsilon_F [1 + (4/3\pi)v^{-1}]$) and the Bose gas of bound pairs (where the right-hand dashed line represents half of the binding energy, $\mu_c \rightarrow -\epsilon_b/2 = -\hbar^2/2ma_F^2 = -\epsilon_F v^2$). Since the vertex function Γ contains the bosonic degrees of freedom and is identified with the boson Greens function, we can read off the effective mass $2m^*$ of the bound pairs from $\Gamma(\mathbf{K}, \Omega_n)$. To do this we take $z_n = i\Omega_n$ as discrete imaginary frequencies and define the related susceptibility $\chi(\mathbf{K}, z)$

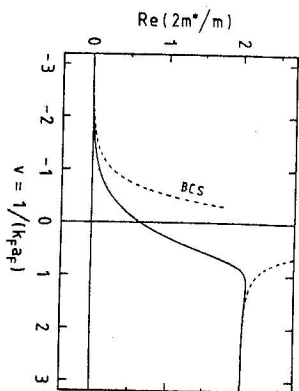


Fig. 5. The real part of the effective boson mass $2m^*$ versus the dimensionless coupling strength v . The full line represents our numerical result. The left-hand dashed line corresponds to the BCS theory. The right-hand dashed line represents the asymptotical strong-coupling result.

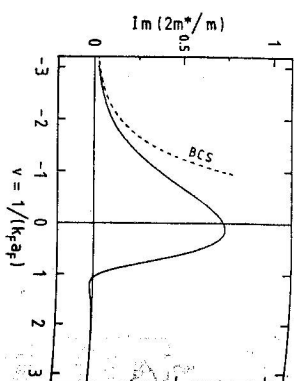


Fig. 6. The imaginary part of the effective boson mass $2m^*$ versus the dimensionless coupling strength v . The full line represents our numerical result. The left-hand dashed line corresponds to the BCS theory. The negative part near $v \approx 1.3$, which would indicate an instability of the system, is presumably a numerical artifact.

for continuous frequencies z as an analytical continuation of $\Gamma(\mathbf{K}, \Omega_n)$ in the upper complex half plane ($\text{Im } z > 0$). The effective mass $2m^*$ is determined by comparing the analytical structure of $\chi(\mathbf{K}, z)$ for $\mathbf{K} \rightarrow 0$ and $z \rightarrow 0$ with the related function of a Bose system. It turns out that this effective mass $2m^*$ is complex and can be identified as the effective mass of a time dependent Ginzburg-Landau equation as in Ref. 11. Our numerical result for $T = T_c$ is shown in Figs. 5 and 6 as full lines. The left-hand dashed lines correspond to the asymptotic result of the BCS theory. In the strong-coupling limit $v \rightarrow +\infty$ nearly all fermions are tightly bound into pairs which behave as bosons of mass $2m^* = 2m$ (twice the fermion mass). As it is expected this limiting result is clearly seen in Figs. 5 and 6. The leading correction is due to the repulsive interaction between the bosons. We have found [1] the asymptotic result $2m^* = 2m[1 + (3\pi)^{-1}v^{-3} + \dots]$ which is real and represented as the right-hand dashed line in Fig. 5.

The effective boson mass $2m^*$ may have an imaginary part which is related to a damping mechanism and to the finite lifetime of the bosons, because the pairs can break up into single fermions. For strong couplings $v \gtrsim +1$ the chemical potential is $\mu_c \lesssim -\epsilon F$ so that in this region nearly all fermions are bound into pairs, while single fermions are rare. Hence the imaginary part of the effective mass $2m^*$ is nearly zero, as it is seen in Fig. 6 for $v \gtrsim +1$. (The small negative imaginary part in Fig. 6 for couplings v between 1.1 and 1.7 is presumably due to a numerical artifact because it would lead to an unphysical instability.) For intermediate and weak couplings $v \lesssim +1$ the system is a mixture of bound pairs and free fermions because of $\mu_c \gtrsim -\epsilon F$. This implies the rather large imaginary part of $2m^*$ which is clearly seen in Fig. 6 for $v \lesssim +1$. Finally, for weak couplings $v \lesssim -1$ the real part becomes negligible compared to the imaginary part because the bound pairs become rare and the fermionic properties become dominant.

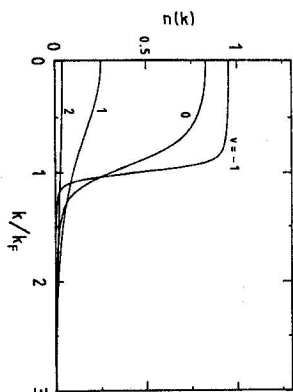


Fig. 7. The fermion occupation number $n(k)$ for various coupling strengths $v = -1, 0, +1, +2$ at $T = T_c$. While for weak coupling $v = -1$ the discontinuity of a Fermi surface at $k = k_F$ is indicated, $n(k)$ is small compared to 1 and similar to a classical distribution function for strong coupling $v = +2$.

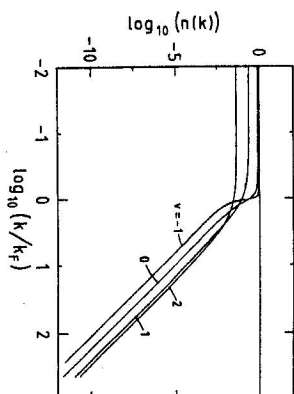


Fig. 8. Double-logarithmic plot of the fermion occupation number $n(k)$ versus k . For large k the power law tails $n(k) \sim k^{-4}$ caused by the bound fermion pairs are clearly seen as straight lines for all couplings $v = -1, 0, +1, +2$.

Until now we have discussed only the bosonic properties of the system which are related to the vertex function Γ . The fermionic properties are included in the fermion Green's function G . Of special interest is the fermion occupation number defined by $n(\mathbf{k}) = -G(\mathbf{k}, \tau = -0)$. The result of our numerical calculations for $T = T_c$ is shown in Fig. 7 for several couplings $v = 1/k_F a_F$. For weak couplings (here $v = -1$) a rather sharp Fermi surface is seen at $k \approx k_F$ which is smeared out more and more for increasing v . For strong couplings (here $v = +1$ and $v = +2$) the occupation number $n(k)$ is small compared to 1 and looks like a classical distribution function. While for an ideal Fermi gas $n(k)$ would decay to zero exponentially for large k , in the present case the bound fermion pairs cause power law tails $n(k) \sim k^{-4}$ for $k \gg k_F$ which are clearly seen as straight lines in the double logarithmic plot (Fig. 8) for all coupling strengths v . In the strong coupling limit the power law tail has been obtained also analytically [1].

5. Conclusions and outlook

While in the limits of weak and strong coupling the mean-field approximation is good and the BCS theory and the theory of the superfluid weakly interacting Bose gas can be recovered, respectively, the numerical analysis has shown that the self-consistency is essential in the crossover region. The self-consistent theory leads to qualitatively new results compared to the previous theories. Since the interaction between the condensed and noncondensed fermion pairs is included in the self-consistent theory, the superfluid transition temperature $T_c(v)$ is a monotonically growing function of the coupling strength v without a maximum in the crossover region. The bound fermion pairs are represented as a power law tail $\sim k^{-4}$ in the fermion occupation number $n(k)$ for large momenta $k \gg k_F$. While for strong couplings $v \gtrsim +1$ the system behaves like a weakly

interacting Bose gas, in the intermediate and weak-coupling range $v \lesssim +1$ the fermion pairs are bosonic quasiparticles with a short lifetime expressed by the large imaginary part of the effective mass $2m^*$.

Our numerical procedure is a powerful method for solving the self-consistent equations, which is not restricted to the superfluid transition at $T = T_c$ but can be applied for arbitrary temperatures T . For future investigations of special interest are thermodynamic quantities like the specific heat $C_v(T)$ and the compressibility $\kappa_T(T)$ at given values of the dimensionless coupling strength $v = 1/k_F a_F$. Furthermore the microscopic functions G and Γ can be used to derive the linearized hydrodynamic equations and to determine transport coefficients like the thermal conductivity $\lambda(T)$ and the shear viscosity $\eta(T)$. This must be done by an analytical continuation analogously as we have shown above, because hydrodynamic equations represent a direct generalization of the time dependent Ginzburg-Landau theory. The resulting physical quantities could then be used for a comparison with experiments.

References

- [1] R. Haussmann: *Z. Phys.* **B91** (1993), 291.
- [2] R. Haussmann: *Phys. Rev.* **B49** (1994), 12975.
- [3] A. L. Fetter, J. D. Walecka: *Quantum theory of many-particle systems* (McGraw-Hill, New York, 1971).
- [4] A. A. Abrikosov, L. P. Gor'kov, I. E. Dzyaloshinskii: *Methods of quantum-field theory in statistical physics* (Dover Publ., New York, 1963).
- [5] A. J. Leggett: in *Modern trends in the theory of condensed matter*, edited by A. Pekalski and J. Przytawska (Springer, Berlin, 1980), p. 13.
- [6] M. Randeria, J.-M. Duan, L.-Y. Shih: *Phys. Rev. Lett.* **62** (1989), 981; *Phys. Rev.* **B41** (1990), 327.
- [7] P. Nozières, S. Schmitt-Rink: *J. Low Temp. Phys.* **59** (1985), 195.
- [8] D. J. Thouless: *Ann. Phys. (N.Y.)* **10** (1960), 553.
- [9] M. Drechsler, W. Zwirger: *Ann. Phys.* **1** (1992), 15.
- [10] S. Stintzing, W. Zwirger (private communication).
- [11] C. A. R. Sá de Melo, M. Randeria, J. R. Engelbrecht: *Phys. Rev. Lett.* **71** (1993), 3202.
- [12] V. M. Galitskii: *Sov. Phys. JETP* **7** (1958), 104.
- [13] L. P. Gor'kov, T. K. Melik-Barkhadarov: *Sov. Phys. JETP* **13** (1961), 1018.
- [14] J. Stoer: *Einführung in die Numerische Mathematik I* (Springer, Berlin, 1983).