MODEL OF THE QUASI-ONE-DIMENSIONAL ELECTRON-ION COULOMB SYSTEM II. DISPERSION RELATIONS

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We study the collective excitions of the quasi-one-dimensional system described by the model Hamiltonian which was derived in the previous paper (Part I). Plasmon and phonon dispersion relations are obtained. The physics we use is essentially the same as in the three-dimensional case. The characteristic one-dimensional effects appear only by the logarithmic singularity of the dielectric function causing a giant anomaly in the renormalized phonom spectrum. This anomaly is accompanied by the lattice instability of the Peierls type.

The transition temperature is calculated in the accompanying paper.

I. INTRODUCTION

Quasi-one-dimensional ($Q1D$) systems are much discussed topics where different models are applied and different physical effects analysed. A detailed understanding of the properties of the $Q1D$ electron-phonon models is of the interest to elucidate the connection between the models and various $Q1D$ real materials. Although much progress has been achieved in the theoretical understanding in recent years [1], many difficult questions remain open [2].

One of the questions to be solved is the problem of the influence of the interplay between electron-electron and electron-phonon interactions on the properties of the $Q1D$ systems. In most theoretical treatises one of these interactions is neglected or treated with uncontrolled approximations. As the $Q1D$ systems can undergo structural phase transitions as a result of both electron-electron and electron-phonon interactions, the consequences of having both interactions together have recently been of considerable interest.

In current models of the electron-phonon systems, the electron-electron interaction is usually parametrised by an on-site (Hubbard) repulsion U between electrons. The effect of U on the ground-state properties has been subject

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of polemics, as the existing results are highly controversial even for simple one-dimensional ($1D$) models of the electron-phonon systems and depend on methods of calculation. Within the mean-field theory, e.g., the SSH model [3] of a $1D$ half-filled band system has a Peierls-dimerized charge-density-wave ground state for an arbitrary strength of an electron-phonon coupling in the absence of an electron-electron interaction. The Hartree—Fock method of the treatment of the SSH model predicts that the $1D$ half-filled system has a Peierls dimerized charge-density-wave ground state as long as the repulsion U is less than a critical value U_c (which depends on the strength of the electron-phonon coupling) and a spin-density-wave ground state for U larger than U_c with a discontinuous transition at U_c [4]. On the other hand, perturbation methods [4, 5] as well as finite chain calculations [4, 6] predict that the dimerization is favoured by an on-site repulsion U. It was also postulated that U has no effect on the properties of a $1D$ system at all [7]. The renormalization-group method predicts a spin-density-wave instability and no charge-density-wave instability in the half-filled electron gas with an on-site repulsion [8]. Similar ambiguities exist also for the influence of a nearest-neighbour repulsion between electrons [5, 9, 10].

In our previous paper [11] (henceforth referred to as paper I) the model Hamiltonian of the $Q1D$ electron-ion Coulomb system was obtained. The quasi-one-dimensionality does not indicate the existence of any mechanism of interchain coupling. It means that the electrons of the system are confined to a tube whose radius is set to be equal to the transverse radius of the ions. The Hamiltonian derived in I is actually the extension of the Fröhlich Hamiltonian to the plasma Hamiltonian. The only interaction involved in the Fröhlich Hamiltonian is the electron-phonon interaction. In addition, the Hamiltonian in I not only involves the electron-ion interaction but the electron-electron interaction as well. Moreover, the strength of both interactions as well as the unrenormalized phonon frequencies are not parametrised but they are properly derived from first principles. The main aim of this paper is to study the influence of both the electron-ion and the electron-electron interactions on the unrenormalized phonon frequencies to get the renormalized ones. In this way, one simultaneously obtains stability conditions for the system, as the squares of the renormalized phonon frequencies should not posses negative values.

It is worth mentioning that the same stability conditions provide a clue to the origin of the structural instability in the $1D$ Fröhlich model [12, 13]. To reveal this instability we employ the expression for the squared renormalized phonon frequencies $\Omega_{ph}^2(q)$ given by

$$\Omega_{ph}^2(q) = \Omega_0^2(q)\left[1 + \frac{2g^2}{\hbar\Omega_0(q)}\,\Lambda_T(q, 0)\right], \tag{1}$$

where $\Omega_0(q)$ is the unrenormalized phonon frequency, g is the strength of the electron-phonon coupling and $\Lambda_T(q, 0)$ is the static Lindhard function. Compared with the known results of the three-dimensional ($3D$) treatment of the Fröhlich Hamiltonian [14, 15], the only difference is the one-dimensionality of $\Lambda_T(q, 0)$. However, the singularity of the $1D$ Lindhard function gives rise to an anomaly in the renormalized phonon spectrum. In the $3D$ case, $\Lambda_T(q, 0)$ has only a smooth anomaly causing the generally shallow anomaly of ordinary metals. In the $1D$ case [16], on the contrary, $\Lambda_T(q, 0)$ at zero temperature is negative and strongly peaked at $q = 2k_f$ (k_f is the Fermi wave vector). Thereupon, $\Omega_{ph}^2(2k_f)$ becomes negative. This violation of the stability condition indicates that the system becomes unstable and leads towards a structural transition.

In this paper, we deal with our model of the $Q1D$ electron-ion Coulomb system. The outline of the paper is as follows: in the next section we briefly sketch the used model of the $Q1D$ electron-ion Coulomb system defined in I. In Sect. III we treat the model without taking into account the effect of periodicity of the lattice and derive the plasmon and phonon dispersion relations in the jellium approximation. The influence of the Umklapp processes on the phonon dispersion relation is considered in Sect. IV.

II. THE HAMILTONIAN

Let us briefly summarize the investigation of the $Q1D$ electron-ion Coulomb system made in I, recapitulating the use notation. The system is composed of electrons and ions interacting according to the Coulomb law. The electrons and ions are confined to a tube formed by a surrounding insulating media. Moreover, the ions of the system are constrained to move only along the tube as we assume that the radius of the tube is equal to the effective transverse radius of the ions. This is not the case of the electrons which can move freely within the tube without any directional restrictions. However, we suppose that all the electrons are at the lowest energy subband related to their motion in the direction perpendicular to the axis of the tube. Furthermore, the electron probability density at the lowest subband is replaced by a constant value.

Using all the above assumptions, it was shown in I that the "*classical*" Hamiltonian of the $Q1D$ electron-ion system has the form:

$$H = E_0 + \frac{1}{2}\sum_k [P(-k)\,P(k) + \Omega_{pl}^2(k)\,Q(-k)\,Q(k)] + \\ + \frac{1}{L}\sum_{\alpha=1}^{N_i}\sum_{j=1}^{N_e}\sum_{q\neq 0} u(q)\,e^{iq(Z_\alpha - z_j)} + \sum_{j=1}^{N_e}\frac{p_j^2}{2m} + \frac{1}{2L}\sum_{j=1}^{N_e}\sum_{\substack{i=1\\ i\neq j}}^{N_e}\sum_{q\neq 0} v(q)\,e^{iq(z_i - z_j)}, \tag{2}$$

where E_0 is the equilibrium position interaction energy of the ions, $Q(k)$ are the normal mode coordinates of the ion oscillations, $P(k)$ is the momentum conjugate to $Q(k)$. The unrenormalized phonon frequencies $\Omega_{pl}(k)$ are defined by

$$\Omega_{pl}^2(k) = \Omega_0^2(k) + \sum_{K_n \neq 0} [\Omega_0^2(k + K_n) - \Omega_0^2(K_n)] \tag{3}$$

with

$$\Omega_0^2(q) = \frac{q^2 w(q)}{aM}, \tag{4}$$

where a is the interionic spacing, L is the longitudinal size of the system and K_n is the reciprocal lattice wave vector.

The functions $w(q)$, $u(q)$, $v(q)$ are the ion-ion, electron-ion and electron-electron interaction matrices, respectively. They obey the relation

$$\frac{u^2(q)}{w(q)\,v(q)} = 1. \tag{5}$$

As usual m, p_j, z_j are the mass, momentum and position of the jth electron and M, Z_α are the mass and position of the αth ion. Its displacement from the equilibrium position $Z_{\alpha 0}$ is given by

$$\delta Z_\alpha = \sum_k \frac{Q(k)}{(MN_i)^{1/2}} e^{ikZ_{\alpha 0}}, \tag{6}$$

where N_i is the number of the ions in the system. It is related to the number of the electrons by $Z^* N_i = N_e$, where Z^* is the effective valence. The sum over k is performed in the first Brillouin zone and that over q in the whole wave space. So far, the only difference between the usual $3D$ plasma Hamiltonian and the present one is the one-dimensionality. However, the interaction matrices significantly differ from their $3D$ counterparts:

$$w(q) = \frac{2Z^{*2}e^2}{\pi\epsilon}\,\gamma(|q|\,r) \tag{7a}$$

$$u(q) = -\frac{2Z^* e^2}{\pi\epsilon}\,\gamma(|q|\,r) \tag{7b}$$

$$v(q) = \frac{2e^2}{\pi\epsilon}\,\gamma(|q|\,r), \tag{7c}$$

where e is the elementary charge, ϵ is the dielectric constant of the surrounding organic media and r is the transverse radius of the ions. The function $\gamma(x)$ is given by

$$\gamma(x) = \frac{1/2 - K_1(x)\,I_1(x)}{x^2}, \tag{8}$$

where $I_1(x)$ and $K_1(x)$ are the modified Bessel functions of the first and second kind, respectively.

Another important result obtained in I is the form of the $Q1D$ Fourier transformation of Poisson's equation:

$$V_s(q) = v(q)\,\delta\varrho(q), \tag{9}$$

where $V_s(q)$ is the Fourier transform of the screening potential and $\delta\varrho(q)$ is the Fourier transform of the induced change in the electron density.

The last result to be mentioned is that $Z^*/2$ represents the degree of the band filling, because

$$k_f = \frac{Z^*\pi}{2a}, \tag{10}$$

where k_f is the Fermi wave vector and π/a is the $1D$ Debye wave vector.

The numerical values of the parameters Z^*, a, ϵ_r (the relative dielectric constant of the surrounding organic media) used throughout the paper are taken from [17] and correspond to a platinum compound like KCP.

In the next section we shall obtain the dispersion relations for the jellium approximation of the ionic behaviour. In this approximation, all effects of periodicity are neglected. As usual, in the expansion of the electron-ion part of the Hamiltonian we keep only the linear term in δZ_α and neglect the next terms. If we further express the terms including the summation over the positions of the electrons in the second quantization, we get

$$\begin{aligned} H = {} & E_0 + \frac{1}{2}\sum_q [P(-q)\,P(q) + \Omega_0^2(q)\,Q(-q)\,Q(q)] - \\ & - \frac{1}{L}\sum_q \sum_{q_1,\,\sigma_1} iqu(-q)\left(\frac{N_i}{M}\right)^{1/2} Q(q)\,c_{\sigma_1}^+(q_1 + q)\,c_{\sigma_1}(q_1) + \\ & + \sum_{q,\,\sigma} E(q)\,c_\sigma^+(q)\,c_\sigma(q) + \frac{1}{2L}\sum_{q\neq 0}\sum_{q_1,\,\sigma_1}\sum_{q_2,\,\sigma_2} \\ & v(q)\,c_{\sigma_1}^+(q_1 - q)\,c_{\sigma_2}^+(q_2 - q)\,c_{\sigma_2}(q_2)\,c_{\sigma_1}(q_1). \end{aligned} \tag{11}$$

As we shall not carry out any explicit Bloch calculations we simply take the energy $E(q)$ appropriate to the free electrons, i.e., $E(q) = \hbar^2 q^2/(2m)$, ($\hbar$ is the Planck constant). Similarly, the operators $c_\sigma(q)$ and $c_\sigma^+(q)$ act to annihilate and to create an electron in the $1D$ plane-wave state with the wave vector q and the spin σ.

III. DISPERSION RELATIONS IN THE JELLIUM APPROXIMATION

The procedure we use in this section is quite similar to that of Pines [18] for the corresponding $3D$ case. The essence of this procedure is deriving equations of motion of the electrons and the ions. Solving these two coupled equations we directly obtain an equation from which the eigenfrequencies of the $Q1D$ system can be calculated.

At first we introduce the operator of an electron-hole pair with the wave vector $-q$ and the spin σ:

$$\varrho_\sigma(q, q_1) = c_\sigma^+(q_1)\, c_\sigma(q_1 + q), \tag{12}$$

whose equation of motion is

$$\begin{aligned} \mathrm{i}\hbar \frac{\partial}{\partial t} \varrho_\sigma(q, q_1) &= [E(q + q_1) - E(q_1)]\, \varrho_\sigma(q, q_1) - \\ &- \frac{1}{L} \sum_{q_2} \mathrm{i} q_2 u(-q_2) \left(\frac{N_i}{M}\right)^{1/2} Q(q_2) [c_\sigma^+(q_1)\, c_\sigma(q + q_1 - q_2) - \\ &- c_\sigma^+(q_1 + q_2)\, c_\sigma(q + q_1)] + \frac{1}{2L} \sum_{q_2 \neq 0} v(q_2) \{\varrho(q_2) [c_\sigma^+(q_1)\, c_\sigma(q + q_1 - q_2) - \\ &- c_\sigma^+(q_1 + q_2)\, c_\sigma(q + q_1)] + [c_\sigma^+(q_1)\, c_\sigma(q + q_1 - q_2) - \\ &- c_\sigma^+(q_1 + q_2)\, c_\sigma(q + q_1)]\, \varrho(q_2)\}, \end{aligned} \tag{13}$$

where $\varrho(q)$ is the electron density fluctuation operator. It can be expressed in terms of $\varrho_\sigma(q, q_1)$ as

$$\varrho(q) = \sum_{q_1, \sigma} \varrho_\sigma(q, q_1). \tag{14}$$

We now make the RPA approximation in (13), i.e. we keep only the terms with $q_2 = q$ and further we replace the operators $c_\sigma^+(q_1)\, c_\sigma(q_1)$ and $c_\sigma^+(q + q_1) \times c_\sigma(q + q_1)$ by their expectation values between the plane-wave states. Then equation (13) reduces to

$$\begin{aligned} \mathrm{i}\hbar \frac{\partial}{\partial t} \varrho_\sigma(q, q_1) &= [E(q + q_1) - E(q_1)]\, \varrho_\sigma(q, q_1) + \\ &+ \frac{1}{L} \left[-\mathrm{i} q u(-q) \left(\frac{N_i}{M}\right)^{1/2} Q(q) + v(q)\, \varrho(q) \right] [f(q_1) - f(q + q_1)], \end{aligned} \tag{15}$$

where $f(q)$ is the average number of the electrons in the plane-wave state, i.e., the Fermi—Dirac distribution function.

If we take the time Fourier transform of (15), we easily obtain

$$\begin{aligned} \varrho_\sigma(q, q_1, \omega) = \frac{1}{L} \Bigg[&-\mathrm{i} q u(-q) \left(\frac{N_i}{M}\right)^{1/2} Q(q, \omega) + \\ &+ v(q)\, \varrho(q, \omega) \Bigg] \left[\frac{f(q_1) - f(q + q_1)}{E(q_1) - E(q + q_1) + \hbar\omega + \mathrm{i}0} \right], \end{aligned} \tag{16}$$

where $\varrho_\sigma(q, q_1, \omega)$, $Q(q, \omega)$, $\varrho(q, \omega)$ are the Fourier transform of $\varrho_\sigma(q, q_1)$, $Q(q)$, and $\varrho(q)$, respectively. The small positive imaginary part in the denominator arises from the choice of the retarded boundary condition.

Summing up over all states (q_1, σ) in equation (16) we obtain

$$\varrho(q, \omega) = \left[-\mathrm{i} q u(-q) \left(\frac{N_i}{M}\right)^{1/2} Q(q, \omega) + v(q)\, \varrho(q, \omega) \right] \Lambda_T^R(q, \omega) \tag{17}$$

where $\Lambda_T^R(q, \omega)$ is the retarded $1D$ Lindhard function defined by

$$\Lambda_T^R(q, \omega) = \frac{1}{L} \sum_{q_1, \sigma} \left[\frac{f(q_1) - f(q + q_1)}{E(q_1) - E(q + q_1) + \hbar\omega + \mathrm{i}0} \right]. \tag{18}$$

In the exact form, it can be calculated only in the case of complete degeneracy, i.e., at zero temperature:

$$\Lambda_0^R(q, \omega) = \frac{m}{\pi\hbar^2 q} \ln \left[\frac{\hbar^2 q^2 (2k_f - q)^2 - 4m^2(\omega + \mathrm{i}0)^2}{\hbar^2 q^2 (2k_f + q)^2 - 4m^2(\omega + \mathrm{i}0)^2} \right]. \tag{19}$$

It must be mentioned here that the imaginary part of $\Lambda_0^R(q, \omega)$ is different from zero only for frequencies which obey the relation

$$\omega_L \leqslant |\omega| \leqslant \omega_R, \tag{20a}$$

where

$$\omega_L = \left| \frac{\hbar q}{2m} (2k_f - |q|) \right| \quad \text{and} \quad \omega_R = \left| \frac{\hbar q}{2m} (2k_f + |q|) \right|, \tag{20b}$$

the energies $\hbar\omega_L$ and $\hbar\omega_R$ represent the minimum and maximum energies for the excitation of an electron-hole pair with the wave vector q. As expected the $1D$ Lindhard function at zero temperature (equation 19) diverges logarithmically at the upper and lower thresholds for an electron-hole pair excitation.

Now, we write down the equation describing the motion of the amplitude $Q(q)$ of the lattice vibration

$$\frac{\partial^2}{\partial t^2} Q(q) + \Omega_0^2(q)\, Q(q) = -\frac{\mathrm{i}}{L} q u(q) \left(\frac{N_i}{M}\right)^{1/2} \varrho(q). \tag{21}$$

The time Fourier transform of (21) has the form

$$[\omega^2 - \Omega_0^2(q)]\, Q(q, \omega) = \frac{\mathrm{i}}{L}\, qu(q)\left(\frac{N_i}{M}\right)^{1/2} \varrho(q, \omega). \tag{22}$$

The two equations (17) and (22) are consistent only if

$$\epsilon_T^R(q, \omega) - \frac{\Omega_a^2(q)}{\omega^2 - \Omega_0^2(q) + \Omega_a^2(q)} = 0, \tag{23}$$

where

$$\Omega_a^2(q) = \frac{q^2 u^2(q)}{aMv(q)} \tag{24}$$

and

$$\epsilon_T^R(q, \omega) = 1 - v(q)\, \Lambda_T^R(q, \omega) \tag{25}$$

is the retarded dielectric function of the $Q1D$ electron Coulomb gas. It was first obtained by Lee and Spector [19]. The left-hand side of equation (23) represents the dielectric function of the $Q1D$ electron-ion Coulomb system in the jellium approximation.

Equation (23) serves for determining the eigenfrequencies of the present model of the $Q1D$ system in jellium approximation. There are two branches to the solution for equation (23). The first is the high-frequency branch (the plasmon mode) in which the electrons and ions oscillate out of phase. Because of their much greater mass the ions are not able to follow the rapid electronic motion, they behave almost as a uniform positive background.

To obtain the plasmon dispersion relation at zero temperature we use equations (19), (25) and rewrite equation (23) in the form

$$\omega^2 = \frac{\hbar^2 q^2}{4m^2}\left(2k_f + q)^2 + 4qk_f\left\{\mathrm{cth}\left[\frac{\pi\hbar^2 q}{2mv(q)}\left(1 - \frac{\Omega_0^2(q)}{\omega^2 - \Omega_0^2(q) + \Omega_a^2(q)}\right)\right] - 1\right\}\right). \tag{26}$$

For a small q ($q \ll r^{-1}$) we can expand the right-hand side of equation (26) and we obtain

$$\omega^2 \simeq \frac{2k_f}{\pi m}\, q^2 v(q)\left[1 + \frac{\Omega_0^2(q)}{\omega^2}\right]. \tag{27}$$

We use relation $\Omega_a^2(q) \simeq \Omega_0^2(q)$ valid for a small q. It follows from the condition of the electrical neutrality of the whole electron-ion system (see I). Moreover, because of equation (5) it is valid for all q in the present model.

The solution of the equation (27) is then

$$\omega_{pl}^2(q) \simeq \frac{2k_f}{\pi m}\, q^2 v(q)\left(1 + \frac{Z^* m}{M}\right). \tag{28}$$

As in the $3D$ system the influence of the ions on the plasmon frequencies is of the order $(Z^* m/M)^{1/2}$, i.e., it is negligible. However, the plasmon frequency spectrum of the $Q1D$ system, in contrast to the $3D$ system, tends to zero as $q \to 0$. This is the consequence of the "*weakness*" of the Coulomb interaction in the $Q1D$ system. It was properly explained in I when we were discussing the unrenormalized phonon dispersion relation.

If we fully neglect the role of the ions in determining the plasmon dispersion relation, we get

$$\omega_{pl}^2(q) = \frac{\hbar^2 q^2}{4m^2}\left((2k_f + q)^2 + 4qk_f\left\{\mathrm{cth}\left[\frac{\pi\hbar^2 q}{2mv(q)}\right] - 1\right\}\right). \tag{29}$$

Fig. 1 shows the plasmon dispersion curve of the present model of the $Q1D$ electron-ion Coulomb system for $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$ m, $\epsilon_r = \epsilon/\epsilon_0 = 2.6$ (ϵ_0 is the dielectric constant of vacuum) and $r = a/2$. The electron-hole pair excitation spectrum is also shown in Fig. 1 (shaded region). The "*hole*" in the spectrum is a general feature of any $Q1D$ electron gas. As a result of this "*hole*", low-energy electron-hole excitations are allowed only for $q \simeq 0$ and $q \simeq 2k_f$ [20].

An interesting feature of the $Q1D$ plasmon dispersion curves is that they never enter the region of electron-hole excitations, i.e., in contrast to $3D$ metals, plasmons in $Q1D$ systems are not Landau damped [20]. This result can easily be seen from equation (29). Remembering that $\mathrm{cth}(x) \geqslant 1$ for all positive x, it follows that $\omega_{pl}(q) \geqslant \omega_R$, the maximum of the electron-hole excitation frequency.

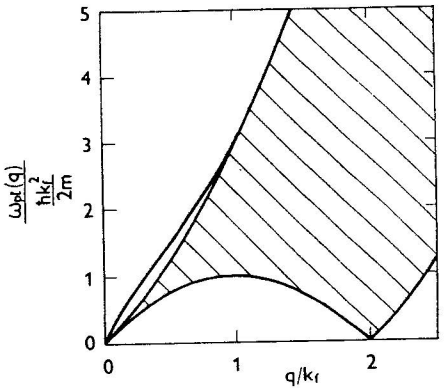

Fig. 1. Plasmon dispersion law of the $Q1D$ electron system.

A similar dependence of $\omega_{pl}(q)$ on q as given by equation (29) was numerically obtained by Lai and Das Sarma [21].

The second branch is a low frequency phonon mode in which the electrons follow the motion of the ions. Since the phonon frequency is generally much smaller than any structure in the electron-hole excitation spectrum, it is sufficient to approximate the phonon dispersion relation by

$$\Omega_{ph}^2(q) = \Omega_0^2(q) - \Omega_a^2(q) + \frac{\Omega_a^2(q)}{\epsilon_T^R(q, 0)}. \tag{30}$$

At zero temperature one has

$$\Omega_{ph}^2(q) = \Omega_0^2(q) - \Omega_a^2(q) + \frac{\Omega_a^2(q)}{1 + \dfrac{2mv(q)}{\pi\hbar^2 q} \ln\left|\dfrac{2k_f + q}{2k_f - q}\right|}. \tag{31}$$

Equation (31) contains a sharp logarithmic singularity at $q = \pm 2k_f$. If $\Omega_0^2(2k_f) < \Omega_a^2(2k_f)$, i.e., if $w(2k_f) < u^2(2k_f)/v(2k_f)$, equation (31) leads to the imaginary phonon frequency at $q = \pm 2k_f$. This unphysical result expresses the Peierls instability of the $Q1D$ system. Such a model of the $Q1D$ electron-ion system in the jellium approximation but interacting via the $3D$ Coulomb interaction was studied by Kurihara [22], Nakane and Takada [23].

However, in the present model $\Omega_a^2(q) = \Omega_0^2(q)$ and the phonon frequencies are real for all q. Though the $2k_f$ phonon frequency becomes soft at zero temperature, i.e., $\Omega_{ph}(2k_f) = 0$, we shall not deal with the phonon dispersion relation obtained from equation (31) any longer. The reason for this is that it seems to be an artefact because the jellium approximation is valid only for small q compared to $2k_f$. To obtain more reliable phonon dispersion relation, the Umklapp processes have to be taken into account. This is done in the next section.

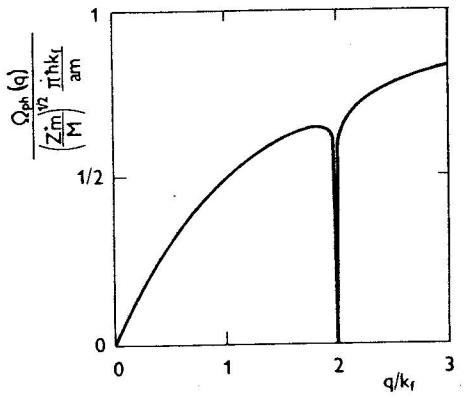

Fig. 2. Phonon dispersion law of the $Q1D$ electron-ion Coulomb system in the jellium approximation.

At the end of this section we mention that for small q equation (31) can be approximated by

$$\Omega_{ph}^2(q) \simeq \frac{Z^* m}{M}\left(\frac{\hbar k_f}{m}\right)^2 q^2. \tag{32}$$

Except for the factor 1/3 we get the expression which is valid for the squared renormalized phonon frequency at small q in the $3D$ case.

The phonon dispersion relation given by equation (31) is shown in Fig. 2 for $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$ m, $\epsilon_r = 2.6$, $r = a/2$.

IV. THE PHONON DISPERSION RELATION INCLUDING THE UMKLAPP PROCESSES

We shall now consider a more comprehensive calculation of the renormalized phonon frequencies, which also includes the Umklapp processes. Our procedure follows that of Callaway [24] for the corresponding $3D$ case. The fundamental point of this procedure is a self-consistent calculation of the change in the electron density $\delta\varrho(z)$. This change, caused by the displacement of the ions alone, influences in turn the motion of the ions. In this way, the electrons which readjust themselves to reduce their effective interaction with the vibrating ions cause a change in the ion-ion interaction. They mediate an effective ion-ion interaction from which the effective dynamical matrix will be obtained.

To determine the effective ion-ion interaction we first consider the change in the wave function of an electron $\delta\psi(q_1, z)$. This change is produced by the change of the electron-ion potential $\delta u(q)$ caused by the displacement of the bare ions and by the change of the electron-electron potential $\delta v(q)$ caused by the readjustment of the electrons alone. Using the first order perturbation theory we have

$$\delta\psi(q_1, z) = \frac{1}{L}\sum_q \left[\frac{\delta u(q) + \delta v(q)}{E(q_1) - E(q + q_1)}\right] \Psi(q + q_1, z). \tag{33}$$

The distortion of the electron wave function gives rise to the change in the electron density. To the first order we get

$$\begin{aligned}\delta\varrho(z) &= \sum_{q_1, \sigma} f(q_1)[\psi^*(q_1, z)\,\delta\psi(q_1, z) + \delta\psi^*(q_1, z)\,\psi(q_1, z)] = \\ &= \frac{1}{L}\sum_q \sum_{q_1, \sigma}\left[\frac{f(q_1) - f(q + q_1)}{E(q_1) - E(q + q_1)}\right][\delta u(q) + \delta v(q)]\,\psi^*(q_1, z)\,\psi(q + q_1, z).\end{aligned} \tag{34}$$

To simplify the calculation we suppose that the unpertubated wave functions

$\psi(q, z)$ are the plane-wave states. Because of this we also have to replace $\delta u(q)$ by the full potential $u(q)$.

If we make the Fourier transform of equation (34), we get with respect to the coordinate z

$$\delta\varrho(q) = [u(q) + \delta v(q)]\, \Lambda_T(q, 0), \tag{35}$$

where

$$\Lambda_T(q, 0) = \frac{1}{L} \sum_{q_1, \sigma} \left[\frac{f(q_1) - f(q + q_1)}{E(q_1) - E(q + q_1)} \right] \tag{36}$$

is the static $1D$ Lindhard function. If we further use the $Q1D$ Fourier transform of Poisson's equation (9) to replace $\delta v(q)$ by $v(q)\, \delta\varrho(q)$, we easily obtain the final expression for the Fourier transform of the change in the electron density:

$$\delta\varrho(q) = \frac{u(q)}{v(q)} \left[\frac{1}{\epsilon_T(q, 0)} - 1 \right], \tag{37}$$

where $\epsilon_T(q, 0) = 1 - v(q)\, \Lambda_T(q, 0)$ is the static dielectric function of the $Q1D$ electron Coulomb gas.

The effective ion-ion interaction H_{ii}^e is a sum of two terms:

$$\begin{aligned} H_{ii}^e &= \frac{1}{2L} \sum_{q \neq 0} \sum_{\alpha=1}^{N_i} \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N_i} \{w(q) + u(q)\, \delta\varrho(q)\} \mathrm{e}^{\mathrm{i}q(Z_\alpha - Z_\beta)} = \\ &= \frac{1}{2L} \sum_{q \neq 0} \sum_{\alpha=1}^{N_i} \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{N_i} \left\{ w(q) + \frac{u^2(q)}{v(q)} \left[\frac{1}{\epsilon_T(q, 0)} - 1 \right] \right\} \mathrm{e}^{\mathrm{i}q(Z_\alpha - Z_\beta)}. \end{aligned} \tag{38}$$

The first term in (38) is the direct ion-ion interaction and the second is the electron-mediated ion-ion interaction.

The calculation of the squared renormalized phonon frequencies is now straightforward, as they are a function of the second derivative of the effective ion-ion interaction:

$$\begin{aligned} \Omega_{ph,\,T}^2(k) &= \frac{1}{M} \sum_{\alpha=1}^{N_i} \left(\frac{\partial^2 H_{ii}^e}{\partial Z_\alpha \partial Z_\beta} \right)_{Z_\beta = Z_{\beta 0}} \mathrm{e}^{\mathrm{i}k(Z_{\alpha 0} - Z_{\beta 0})} = \\ &= \Omega_0^2(k) + \sum_{K_n \neq 0} [\Omega_0^2(k + K_n) - \Omega_0^2(K_n)] - \\ &\quad - \Omega_a^2(k) - \sum_{K_n \neq 0} [\Omega_a^2(k + K_n) - \Omega_a^2(K_n)] + \\ &\quad + \frac{\Omega_a^2(k)}{\epsilon_T(k, 0)} + \sum_{K_n \neq 0} \left[\frac{\Omega_a^2(k + K_n)}{\epsilon_T(k + K_n, 0)} - \frac{\Omega_a^2(K_n)}{\epsilon_T(K_n, 0)} \right]. \end{aligned} \tag{39}$$

The term containing Ω_0 is the contribution of the ions of the lattice and the term containing Ω_a is the contribution of the electrons determined by the properties of the electrons in the periodic field of the lattice. The function $\Omega_{ph,\,T}^2(k)$ is an even and periodic function with the period of the reciprocal lattice wave vector as it could be expected.

The preceding calculations should be improved in several respects. We have treated the electron-electron interaction in a simple way, amounting to a Hartree approximation. Each electron has been assumed to move independently except in an average field produced by the other electrons. Neither exchange nor more detailed correlation effects have been taken into account. However, concerning the renormalized phonon frequencies we confine ourselves to equation (39) as the improvement of the calculation is not an easy task, especially for $Q1D$ systems.

In the present model, $\Omega_a^2(q) = \Omega_0^2(q)$ and equation (39) reduces to

$$\Omega_{ph,\,T}^2(k) = \frac{\Omega_0^2(k)}{\epsilon_T(k, 0)} + \sum_{K_n \neq 0} \left[\frac{\Omega_0^2(k + K_n)}{\epsilon_T(k + K_n, 0)} - \frac{\Omega_0^2(K_n)}{\epsilon_T(K_n, 0)} \right]. \tag{40}$$

For small k, we have the following approximation

$$\Omega_{ph,\,T}^2(k) = \frac{\Omega_0^2(k)}{\epsilon_T(k, 0)} + k^2 \sum_{K_m > 0} \frac{\partial^2}{\partial K_n^2} \left[\frac{\Omega_0^2(K_n)}{\epsilon_T(K_n, 0)} \right] = \frac{Z^* m}{M} \left(\frac{\hbar k_f}{m} \right)^2 k^2 \Phi_T(r/a), \tag{41}$$

where at zero temperature

$$\Phi_0(r/a) = 1 + \frac{mM}{Z^* \hbar^2 k_f^2} \sum_{K_n > 0} \frac{\partial^2}{\partial K_n^2} \left[\frac{\Omega_0^2(K_n)}{\epsilon_0(K_n, 0)} \right]. \tag{42}$$

As expected, $\Omega_{ph,\,T}(k)$ is proportional to k. In screening the ionic motion, the electrons act to reduce the long wavelength phonon frequency from $\Omega_{pl}(k)$ to a linear function k. The plot of the function $\Phi_0(x)$ is shown in Fig. 3. As before, we have chosen $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$ m, $\epsilon_r = 2.6$.

The condition for the dynamical stability of the lattice requires $\Omega_{ph,\,T}^2(k) > 0$. However, it can be seen in Fig. 3 that there is a region of values of the parameter x ($x \approx 0 \div x_0$) in which the function $\Phi_0(x)$ is negative. The negative values of $\Phi_0(x)$ yield negative values of $\Omega_{ph,\,T}^2(k)$ given by (41). This indicates the lattice instability of the present model of the $Q1D$ system with the values of the parameters Z^*, a, ϵ_r given above and $r < x_0 a$. In this section, we also show that the lattice is unstable not only for $r < x_0 a$ but for all physically interesting values of parameter r (i.e., for $r < a$).

The plot of the squared renormalized phonon frequency at zero temperature as a function of the wave vector is shown in Fig. 4a and Fig. 4b for two different

values of the transverse radius of the ions. Again $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$ m, $\epsilon_r = 2.6$, $r = 0.5a$ and $r = 0.9a$, respectively.

There is a giant anomaly in the renormalized phonon spectrum, which appears in the wave vectors $q = \pm(2k_f + K_n)$. For our choice of the parameter Z^*, the wave vector $k = K_1 - 2k_f = \pi a/3$ is the only positive wave vector in the first Brillouin zone in which the anomaly appears). The origin of this anomaly is the singularity of the $1D$ Lindhard function at $2k_f$ caused by the sharpness of the Fermi surface. If the Fermi surface is sharp, one has a different contribution to $\Lambda_T(q, 0)$ from an electron-hole pair excitation when $q > 2k_f$.

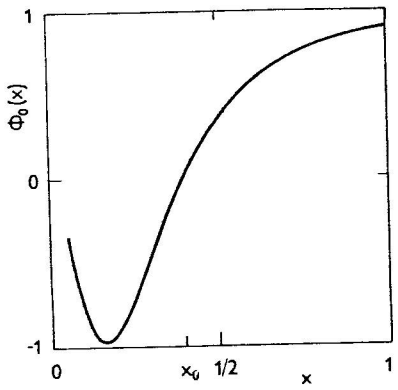

Fig. 3. The plot of the function $\Phi_0(x)$ as defined by equation (42).

Namely, for such wave vector transfers it is no longer possible to excite an electron-hole pair. Moreover, in the $1D$ case, since the Fermi surface is restricted to a pair of points such as $q_1 = \pm 2k_f$, the nesting condition $E(q_1) - E(q_1 + 2k_f) = 0$ (the denominator of equation (36)) is satisfied over the entire Fermi surface resulting in a logarithmic singularity of $\Lambda_0(2k_f, 0)$. Thus, one expects that the corresponding anomaly in the phonon spectrum is a characteristic of all $Q1D$ electron-ion systems, and is not simply a characteristic of the method of the calculation (the RPA approximation in our case).

In the present model the phonon anomaly is so giant that the condition of the lattice stability $\Omega^2_{ph,T}(k) > 0$ is violated. The squares of the phonon frequencies in Fig. 4a and Fig. 4b possess negative values leading to imaginary phonon frequencies. This unphysical result indicates the lattice instability of the $Q1D$ system with respect to the Peierls transition accompanied by the formation of charge-density-waves. Fig. 5 shows the squared renormalized phonon frequency at the wave vector $2k_f$ as a function of the transverse radius of the ions. Again the values of the parameters Z^*, a, ϵ_r are chosen as before. As the squared

renormalized phonon frequency $\Omega^2_{ph,0}(2k_f)$ is negative over all the region of physically interesting values of the parameter r, we conclude that the present model of the $Q1D$ electron-ion Coulomb system with the parameter Z^*, a, ϵ_r given above always exhibits the lattice instability of the Peierls type.

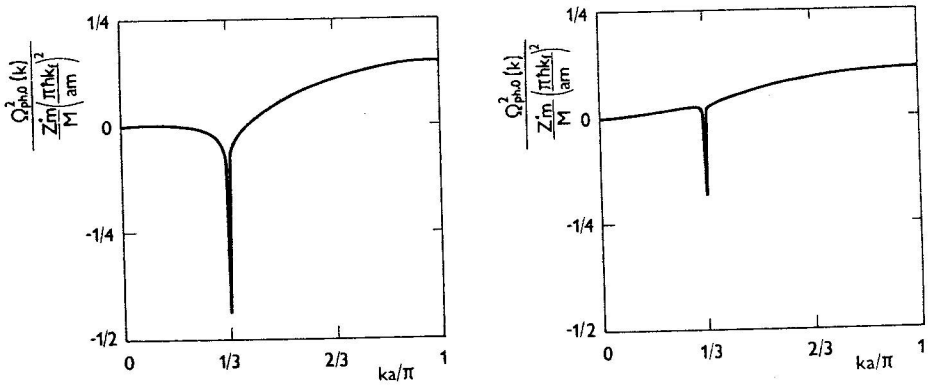

Fig. 4. Squared renormalized phonon frequencies of the $Q1D$ electron-ion Coulomb system as a function of the wave vector, a) for $r = 0.5a$ and b) for $r = 0.9a$.

However, with increasing temperature the singularity of $\Lambda_0(2k_f, 0)$ is smoothed out by the smearing of the Fermi—Dirac distribution function (the numerator of equation (36)). This results only in a sharp peak of $\Lambda_T(2k_f, 0)$, which progresively weakens with increasing temperature. Consequently, the phonon anomaly at $2k_f$ becomes less giant and above some temperature T_P the squares of the renormalized phonon frequencies do not possess negative values any more. The temperature T_P (called the transition temperature) is calculated in our accompanying paper.

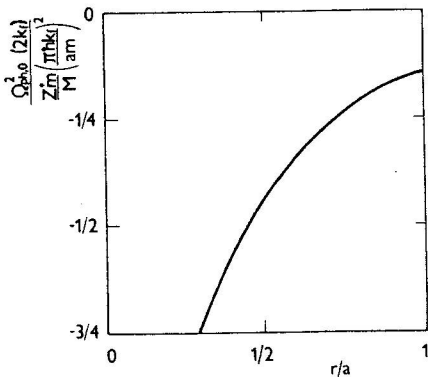

Fig. 5. Squared renormalized phonon frequency at $2k_f$ as a function of the transverse radius of the ions.

V. CONCLUSIONS

In the present paper we have dealt in detail with the dispersion relations of two types of excitations of the $Q1D$ electron-ion Coulomb system. As in every electron-ion Coulomb system, there are also in the present $Q1D$ system three types of elementary excitations: plasmons, phonons and quasi-particles.

Plasmons are collective excitations of electron density. Since every electron feels the force caused by every other electron, however distant it may be, each electron is correlated with all the other electrons. Most of the energy of the longrange part of the Coulomb interaction goes into a correlated collective motion of the electrons in which their density fluctuates. Such an oscillation, a plasma oscillation, has a high energy of excitation and usually is not excited. Therefore, it can be ignored for most phenomena.

Phonons are normal modes of vibrations of the ions which make up the lattice. The original bare phonon frequencies, calculated using only the direct ion-ion interaction, are screened due to the electron-ion and electron-electron interactions. In the $Q1D$ system the screening not only shifts the phonon frequency from $\Omega_{pl}(k)$ to a linear function of small k but causes a giant anomaly at $2k_f$ as well. This anomaly can be regarded as the result of the effects of the electron-ion and electron-electron interactions on the unrenormalized phonon frequencies. Because of the perfect nesting of the Fermi surface in the $1D$ electron system, this anomaly is so giant that at some temperature the softening of the phonon frequencies appears followed by the lattice instability below this temperature. We have already mentioned that our accompanying paper deals with the calculation of this transition temperature.

Quasi-particles of the present model of the $Q1D$ system are the excitations of the electron system. They have been mentioned only very briefly throughout this paper. Moreover, they are been described only in terms of single electron excitations. But it is necessary to point out that the electronic spectrum is influenced by the appearance of the lattice instability. Studying the $1D$ system described by the Fröhlich Hamiltonian, Lee at al. [25] showed that a gap appears in the electronic spectrum. In one of our next papers we intend to deal also with this problem.

At the end of this paper, we emphasize an important circumstance. Although we have revealed the existence of the same lattice instability (the Kohn anomaly) as known in the $1D$ Fröhlich model there is still an advantage of the present model when compared with the Fröhlich model. Namely, the present model was derived from first principles.

The main shortcoming of the Fröhlich model, as it was pointed out by Maksimov and Khomskii [15], is the absence of a consistent method of allowing for the electron-electron Coulomb interaction. When the Fröhlich Hamiltonian is being written down it is usually assumed that the strength of the electron-phonon coupling and the phonon frequencies should be taken with an allowance for the screening of the electron-ion and ion-ion interactions by the electrons. However, there does not exist any consistent method of division of the Coulomb interaction into the part that has already been taken into account in the bare values of the constant of the Fröhlich Hamiltonian and the part that subsequently manifests itself in the renormalization of the bare phonon frequencies as a result of the electron-ion interaction. Thus, one has to be careful while drawing conclusions from the Fröhlich model as the electron-ion interaction is taken into account in two steps: first, in the choice of the bare phonon spectrum, secondly, in the computation of the renormalization of the phonons [26].

As mentioned, within the framework of the Fröhlich model the anomaly in the spectrum of the actually observable phonons (equation (1)) and the lattice instability are related only to the change that occurs in the effective inter-ion interaction as a result of the polarization of the electrons [15]. On the other hand, as can be seen from the treatment in this paper, the present model of the $Q1D$ system yields the other interpretation of the lattice instability. First, we introduced the unrenormalized phonons, i.e., the plasma oscillations of the ions. The subsequent allowance for the interaction of the unrenormalized phonons with the electrons leads to their renormalization, which yields the renormalized spectrum of the phonons excitations of the $Q1D$ system (equation (39)). The onset of the lattice instability and the appearance of negative values in the renormalized phonon spectrum can thus be regarded as the result of the effect of the mutual interplay between the electron-ion and electron-electron interactions on the spectrum of the unrenormalized phonon frequencies.

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МОДЕЛЬ КВАЗИОДНОМЕРНОЙ ЭЛЕКТРОН-ИОННОЙ КУЛОНОВСКОЙ СИСТЕМЫ II. ДИСПЕРСИОННЫЕ СООТНОШЕНИЯ

В работе рассмотриваются коллективные возбуждения квазиодномерной системы описываемой модельным гамильтонияном который был выведен в предыдущей статье (Часть I). Получены дисперсионные соотношения для плазмонов и фононов. Физика, которой пользуемся в сущности та же самая как в трехмерном случае. Характерные одномерные эффекты появляются только посредством логарифмической сингулярности диэлектрической проницаемости, которая вызывает большую аномалию в перенормированном фононном спектре. Эта аномалия сопровождаемая решеточной неустойчивостью пайерлсовского типа.

Температура перехода вычисляется в сопровождаемой статье.