acta phys. slov. 38 (1988), No. 1

MODEL OF THE QUASI-ONE-DIMENSIONAL ELECTRON-ION COULOMB SYSTEM I. GENERAL FORMULATION

JANETKA, I.,[1] Bratislava

The Hamiltonian of the quasi-one-dimensional system is derived from first principles. The electrons and ions of the system are supposed to interact only through the pure Coulomb interaction. We find that the interaction matrices have logarithmic divergence in the zero wave vector limit. This is the consequence of the long-range nature of the Coulomb potential. Owing to the logarithmic character of the divergence the unrenormalized phonon frequency is equal to zero as the wave vector is approaching zero. The dependence of the Fourier transform of the Coulomb potential on the transverse size of the system is also discussed in detail. We further derive the quasi-one-dimensional Fourier transform of Poisson's equation.

The influence of both electron-ion and electron-electron interactions on phonon frequencies will be studied in a forthcoming paper.

I. INTRODUCTION

Many years ago it was recognized that the behaviour of quasi-one-dimensional (Q1D) solids must differ dramatically from that of their three-dimensional (3D) counterparts [1]. The interest in the variety of exciting properties of this class of solids has increased with the development of materials whose microscopic structures consist of well-separated, parallel, metallic chains along which electrons propagate essentially in one dimension.

There are two different theoretical methods of the mathematical description of these systems. In one, the starting Hamiltonian is the Fröhlich Hamiltonian [2, 3]. This model usually describes a system of conduction electrons forced to move along parallel chains without a chance of hopping from chain to chain, interacting with phonons. The intrachain electron-electron interaction is not explicitly considered in this model. The total electron-phonon Hamiltonian is introduced intuitively. There is no rigorous procedure based on the exact analysis of the electron-ion system of the metal for deriving this Hamiltonian.

[1] Slovak Academy of Sciences, Institute of Electrical Engineering, Dúbravská cesta 9, 842 39 BRATISLAVA, Czechoslovakia.

This model is often used for describing the structural transition caused by the electron-phonon interaction.

In the other method, only the electron system is considered, since the particular features of the one-dimensional (1D) electron gas themselves explain many properties of the Q1D conductors. Even if only the electron system is considered, there are still two different approaches. For a description of systems in which the conductivity along the chains is almost metallic, a 1D Fermi gas model with two-body interactions can be used [4]. The elementary interaction processes which are permitted in the 1D Fermi gas model consist of the excitations of a particle-hole pair of small momentum and large momentum. The strictly 1D Fermi model has been extended to a set of coupled chains. There are two possible mechanisms of the interchain interaction: the interchain scattering of electrons [4—7] and direct hopping (tunelling) of electrons from chain to chain [4, 8, 9]. This extended model provides a more realistic image of behaviour of Q1D conductors. In the other approach, which is more suitable for nonconducting systems, a Hubbard Hamiltonian with strong intra-atomic correlation is used [10, 11]. These two approaches are essentially the limiting cases of a general model of interacting electrons written in different representations (momentum or site representation).

Very recently, models trying to unify both methods of the description have appeared. These models describe a Q1D gas of electrons not only interacting mutually through two-body interaction but with phonons as as well. However, in all these models the strengths of the electron-electron, electron- ion and ion-ion intrachain interactions are either parametrised by constants [12—14] or replaced by the 3D Fourier transforms of the corresponding Coulomb potentials [15, 16]. The reason for this is that in a strictly 1D system the Fourier transform of the bare Coulomb potential has a logarithmic singularity. This singularity causes serious difficulties in trying to employ a 1D electron ion Coulomb Hamiltonian. To avoid the logarithmic singularity of the 1D Fourier transform of the bare Coulomb potential we assume that we have a Q1D system which consists of the electrons and ions interacting via the bare Coulomb interaction. The quasi-one-dimensionality means that the electrons and ions are confined to a tube which is formed by a surrounding homogeneous insulating medium. The radius of the tube is supposed to be equal to the effective transverse radius of the ions.

In this paper we present the derivation of the Hamiltonian for a Q1D electron-ion system interacting via the bare Coulomb interaction. The paper is organized as follows: the precise statement of the model is made in Sect. II, where the Hamiltonian is obtained. In Sect. III the Fourier transform of the interaction potential in the present Q1D Coulomb system is discussed, Sect. IV is devoted to the derivation of the Q1D Fourier transform of Poisson's equation and in Sect. V we calculate the unrenormalized phonon frequencies.

II. THE HAMILTONIAN

As mentioned the present Q1D system consists of the electrons and ions confined to a tube of the length L and the radius r. The total Hamiltonian H of any electron-ion system consists of three main parts:

$$H = H_i + H_e + H_{ei} \tag{1}$$

where H_i, H_e, H_{ei} are the ion, electron and electron-ion parts of the total Hamiltonian, respectively.

Let us begin the investigation of the Q1D electron-ion system with the simplification of the ion part of the Hamiltonian. This has the general form:

$$H_i = \sum_{\alpha=1}^{N_i} \frac{P_\alpha^2}{2M} + \frac{1}{2} \sum_{\alpha=1}^{N_i} \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_i} W(Z_\alpha, Z_\beta) \tag{2}$$

where M, Z_α, P_α are the mass, position and momentum of the α-th ion, N_i is the number of the ions in the system. The mutual interaction between the α-th and the β-th ion is denoted by $W(Z_\alpha, Z_\beta)$.

We suppose that each ion of the system possesses a rotational symmetry with a rotational axis identical with the axis of the tube, the electrons and ions are confined to. We further suppose that every ion has the shape of an oblate ellipsoid of evolution whose longer axis is equal to the radius of the tube. Because of this ions can move only along the tube. The longitudinal radius of the ions has to be less than half of the interionic spacing in order that the ions cannot overlap. As a matter of fact, we shall later neglect the longitudinal size of the ions.

The bare ion-ion Coulomb interaction is:

$$W(Z_\alpha, Z_\beta) = \iint w(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) \frac{\mathrm{d}V \mathrm{d}V'}{V^2} \tag{3}$$

with the intergrand:

$$w(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) = \frac{Z^{*2} e^2}{4\pi\epsilon |\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta|} \tag{4}$$

where $\boldsymbol{R}_\alpha = (\boldsymbol{R}_\perp, Z_\alpha + z)$, $\boldsymbol{R}_\beta = (\boldsymbol{R}'_\perp, Z_\beta + z')$, V is the volume of an ion, Z^* is the effective valence (we suppose that $Z^* \approx 0 \div 2$), e is the elementary charge and ϵ is the dielectric constant of the surrounding organic medium (typical

values of the relative dielectric constant lie in the region $\epsilon_r \approx 2$—3). The integrations are performed over the volume of the α-th and the β-th ion.

The function $w(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta)$ can be expanded in the following form [17, 18]:

$$w(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) = \frac{Z^{*2} e^2}{2\pi\epsilon L} \sum_{q\neq 0} K_0(|q|\, \boldsymbol{R}_\perp - \boldsymbol{R}'_\perp)\, \mathrm{e}^{iq(Z_\alpha - Z_\beta + z - z')} \tag{5}$$

where $q = 2\pi n/L$ and n is an integer, L is the longitudinal size of the system, $K_n(x)$ is the modified Bessel function of the second kind of the order n and argument x. The term with $q = 0$ in (5) is omitted because the ions are supposed to be immersed in a uniform background of a negative charge.

If we neglect the longitudinal size of the ions, the expression (3) gets the form:

$$W(Z_\alpha, Z_\beta) = \frac{1}{L} \sum_{q\neq 0} w(q)\, \mathrm{e}^{iq(Z_\alpha - Z_\beta)} \tag{6}$$

where

$$w(q) = \frac{Z^{*2} e^2}{2\pi\epsilon} \iint K_0(|q|\, \boldsymbol{R}_\perp - \boldsymbol{R}'_\perp) \frac{\mathrm{d}^2 R_\perp\, \mathrm{d}^2 R'_\perp}{(\pi r^2)^2} \tag{7}$$

and r is the size of the transverse radius of the ions. The integrations in (7) are performed inside the circle of the radius r. If we use polar coordinates and Graf's addition theorem for $K_0(x)$ [17, 18], we obtain:

$$w(q) = \frac{2Z^{*2} e^2}{\pi\epsilon r^4} \left\{ \int_0^r \mathrm{d}R \left[\int_0^R RR' K_0(|q|\, R)\, I_0(|q|\, R')\, \mathrm{d}R' + \right.\right.$$
$$\left.\left. + \int_R^r RR' I_0(|q|\, R)\, K_0(|q|\, R')\, \mathrm{d}R' \right] \right\} \tag{8}$$

where $I_n(x)$ is the modified Bessel function of the first kind of the order n and argument x. The integration in (8) can easily be performed and we get:

$$w((q) = \frac{2Z^{*2} e^2}{\pi\epsilon} \gamma(|q|\, r) \tag{9}$$

where

$$\gamma(x) = \frac{1/2 - K_1(x)\, I_1(x)}{x^2} \tag{10}$$

Hence, the ion part of the total Hamiltonian is:

$$H_i = \sum_{\alpha=1}^{N_i} \frac{P_\alpha^2}{2M} + \frac{1}{2L} \sum_{\alpha=1}^{N_i} \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_i} \sum_{q\neq 0} w(q)\, \mathrm{e}^{iq(Z_\alpha - Z_\beta)} \tag{11}$$

Now, we shall try to simplify the electron part of the Hamiltonian. As the electrons are confined to a tube (i.e., they are free to move along the axis of the tube but their motion in the transverse direction is confined to the interior of the circle), the electron part of the Hamiltonian can be expressed in the form:

$$H_e = H_{e\parallel} + H_{e\perp} + H_{ee} \tag{12}$$

where

$$H_{e\parallel} = \sum_{j=1}^{N_e} \frac{p_j^2}{2m} \tag{13}$$

$$H_{e\perp} = \sum_{j=1}^{N_e} \frac{\boldsymbol{p}_{j\perp}^2}{2m} + U(\boldsymbol{r}_{j\perp}) \tag{14}$$

$$H_{ee} = \frac{1}{2} \sum_{j=1}^{N_e} \sum_{\substack{i=1\\ i\neq j}}^{N_e} \frac{e^2}{4\pi\epsilon |\boldsymbol{r}_i - \boldsymbol{r}_j|} = \frac{1}{2L} \sum_{j=1}^{N_e} \sum_{\substack{i=1\\ i\neq j}}^{N_e} \sum_{q\neq} \frac{e^2}{2\pi\epsilon} K_0(|q|\,|\boldsymbol{r}_{j\perp} - \boldsymbol{r}_{i\perp}|)\, e^{iq(z_j - z_i)}. \tag{15}$$

Here m is the electron mass, p_j and $\boldsymbol{p}_{j\perp}$ are the momenta of the j-th electron in the longitudinal and in the transverse directions, respectively, $r_j = (\boldsymbol{r}_{j\perp}, z_j)$ is the position of the j-th electron, N_e is the number of the electrons in the system. The potential $U(\boldsymbol{r}_\perp)$ ensures that the electrons cannot escape from the tube, because

$$U(\boldsymbol{r}_\perp) = \begin{cases} 0 & \text{for} \quad |\boldsymbol{r}_\perp| < r \\ \infty & \text{for} \quad |\boldsymbol{r}_\perp| > r \end{cases} \tag{16}$$

The term with $q = 0$ in (15) is again omitted as the electrons are immersed in a uniform background of a positive charge. As known, the wave eigenfunctions in polar coordinates $r_\perp$, φ and the energy eigenvalues of the Hamiltonian $H_{e\perp}$ are:

$$\psi_{l,n}(r_\perp, \varphi) = \begin{cases} \dfrac{J_k(k_{l,n} r_\perp)}{(\pi r^2)^{1/2} J_{l+1}(k_{l,n} r)} e^{il\varphi} & \text{for } r_\perp < r \\ 0 & \text{for } r_\perp > r \end{cases} \tag{17}$$

$$E_{l,n} = \frac{\hbar^2 k_{l,n}^2}{2m} \tag{18}$$

where $J_l(x)$ is the Bessel function of the order l and argument x, $k_{l,n}$ is related to the n-th zero of the Bessel function of the order l, i.e., $J_l(k_{l,n} r) = 0$ and $\hbar$ is the Planck constant.

To rewrite the electron-electron part of the Hamiltonian (equation (15)) in the second quantization, it is necessary to calculate the following integral:

$$\iint d^2 r_\perp\, d^2 r'_\perp\, \psi^*_{l_1,n_1}(r_\perp, \varphi)\, \psi^*_{l_2,n_2}(\boldsymbol{r}', \varphi')\, K_0(|q|\,|\boldsymbol{r}_\perp - \boldsymbol{r}'| \times$$
$$\times\, \psi_{l_3,n_3}(\boldsymbol{r}', \varphi')\, \psi_{l_4,n_4}(r_\perp, \varphi). \tag{19}$$

In trying to evaluate such integrals some complications arise. To avoid them we shall always consider that all the electrons of the system are at the lowest energy level.

The difference between two energy levels of an electron confined to the interior of the circle of the radius r can be estimated by $\delta E \approx \hbar^2/(2mr^2)$. We assume that the temperature T is so low that the temperature fluctuation cannot cause transitions of the electrons from the lowest energy level to a higher one, i.e. $k_B T \ll \delta E$ (k_B is the Boltzmann constant). Therefore, we assume that only the ground state subband related to the transverse motion is occupied by electrons. We also replace the ground state electron probability density by a constant [19]:

$$\psi^*_{0,1}(r_\perp, \varphi)\, \psi_{0,1}(r, \varphi) = \begin{cases} \dfrac{1}{\pi r^2} & \text{for } r_\perp < r \\ 0 & \text{for } r_\perp > r \end{cases} \tag{20}$$

Now integrals in (19) can be easily evaluated. In accordance with the above assumptions the only integral different from zero is that with $l_1 = l_2 = l_3 = l_4 = 0$ and $n_1 = n_2 = n_3 = n_4 = 1$ and its value is $4\gamma(|q|\, r)$.

Then the electron part of the total Hamiltonian can be rewritten in the form

$$H_e = \sum_{j=1}^{N_e} \frac{p_j^2}{2m} + \frac{1}{2L} \sum_{j=1}^{N_e} \sum_{\substack{i=1\\ i\neq j}}^{N_e} \sum_{q\neq 0} v(q)\, e^{iq(z_j - z_i)} \tag{21}$$

where

$$v(q) = \frac{2e^2}{\pi\epsilon} \gamma(|q|\, r). \tag{22}$$

The last part of the total Hamiltonian to be simplified is the electron ion part:

$$H_{ei} = \sum_{\alpha=1}^{N_i} \sum_{j=1}^{N_e} U(Z_\alpha, \boldsymbol{r}_j) \tag{23}$$

where $U(Z_\alpha, \boldsymbol{r}_j)$ specifies the interaction between the α-th ion and the j-th electron and can be expressed as:

$$U(Z_\alpha, \boldsymbol{r}_j) = \int u(\boldsymbol{R}_\alpha, \boldsymbol{r}_j) \frac{dV}{V} \tag{24}$$

with the integrand:

$$u(\boldsymbol{R}_\alpha, \boldsymbol{r}_j) = -\frac{Z^* e^2}{4\pi\in|\boldsymbol{R}_\alpha - \boldsymbol{r}_j|} \tag{25}$$

The integration in (24) is performed over the body of the α-th ion. We assume that the interaction of the electron with the ion is not affected by the motion of the ion and that it is of the form of the pure Coulomb interaction.

If we make the same approximation as at the simplification of the ion and electron parts of the Hamiltonian (i.e., we neglect the longitudinal size of the ions and assume that all the electrons occupy the ground state subband related to the transverse motion), we get:

$$H_{ei} = \frac{1}{L}\sum_{\alpha=1}^{N_i}\sum_{j=1}^{N_e}\sum_{q\neq 0} u(q)\, e^{iq(Z_\alpha - z_j)} \tag{26}$$

where

$$u(q) = -\frac{2Z^* e^2}{\pi\in}\gamma(|q|\, r). \tag{27}$$

Again, we omit the term with $q = 0$ because we suppose that the interaction of each electron with a uniform positive charge distribution is subtracted from the electron-ion interaction. We have already susbtracted the self-energy of a uniform negative charge distribution from the electron-electron interaction and the self-energy of a uniform positive charge distribution from the ion-ion interaction. The sum of these three corrections adds to zero so that the total Hamiltonian is unchanged. The absence of the term with $q = 0$ in the total Hamiltonian is the consequence of the electrical neutrality of the present electron-ion system.

From the condition of the electrical neutrality of the system we can obtain the expression connecting the Fermi wave vector with the Debye wave vector. As the whole charge of the electrically neutral system is equal to zero, the equation $Z^* N_i = N_e$ is valid. It is obvious that $N_i = L/a$ and $N_e = 2Lk_f/\pi$, where a is the interionic spacing and k_f is the Fermi wave vector. Combining the previous equations we obtain:

$$k_f = \frac{Z^*\pi}{2a} \tag{28}$$

Therefore, the parameter $Z^*/2$ expresses the degree of band filling because π/a is the $1D$ Debye wave vector. As a matter of fact, the values of k_f and are a known from experiments and equation (28) can be used to calculate the parameter Z^*.

The condition of the electrical neutrality is often represented by a relation among $v(q)$, $u(q)$ and $w(q)$ [20], namely:

$$\lim_{q\to 0}\frac{u^2(q)}{w(q)\, v(q)} = 1. \tag{29}$$

As in the present model the electron-ion potential is the pure Coulomb potential, the relationship (29) is not only valid in the limit $q \to 0$ but for all values of q.

III. THE INTERACTION POTENTIAL IN THE $Q1D$ COULOMB SYSTEM

The function

$$\gamma(x) = \frac{1/2 - K_1(x)\, I_1(x)}{x^2} \tag{30}$$

which gives the $Q1D$ Fourier transform of the Coulomb potential

$$v(q) = \frac{2e^2}{\pi\in}\gamma(|q|\, r) \tag{31}$$

was first defined by Lee and Spector [19]. It is shown in Fig. 1. In the limit $x \to 0$ one has:

$$\gamma(x) = -\frac{1}{4}\ln\left(\frac{x}{2}\right) + \ldots \tag{32}$$

Hence, the $Q1D$ Fourier transform of the Coulomb potential diverges logarithmically as either the transverse size of the system or the wave vector are approaching zero. The divergence at $r = 0$ expresses the logarithmic singularity of the $1D$ Fourier transform of the bare Coulomb interaction and that at $q = 0$ is the consequence of the long-range nature of the Coulomb interaction.

In the limit of large x, the following expansion holds:

$$\gamma(x) = \frac{1}{2x^2} - \frac{1}{2x^3} + \ldots \tag{33}$$

Therefore, in the limit $q \to \infty$ we get the expected form of the $Q1D$ Fourier transform of the Coulomb potential [21]:

$$v(q) = \frac{1}{\pi r^2}\left(\frac{e^2}{\in q^2}\right) + \ldots \tag{34}$$

The expression in the round brackets of equation (34) is the known form of the $3D$ Fourier transform of the Coulomb potential.

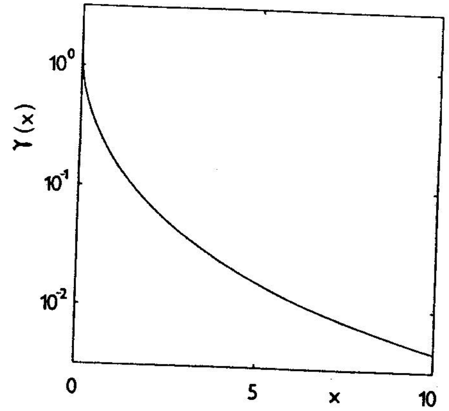

Fig. 1. The plot of the function $\gamma(x)$ as defined by equation (30).

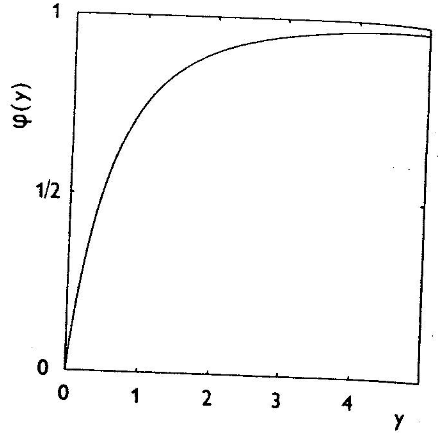

Fig. 2. The plot of the function $\varphi(y)$ as defined by equation (36).

If we make the inverse $1D$ Fourier transform of $v(q)$, we obtain:

$$V(z) = \frac{e^2}{4\pi\epsilon|z|}\varphi\left(\frac{z}{r}\right) \tag{35}$$

where $V(z)$ denotes the $1D$ Fourier transform of $v(q)$ and

$$\varphi(y) = \frac{8|y|}{\pi}\int_0^\infty \gamma(x)\cos(xy)\,\mathrm{d}x\,. \tag{36}$$

It can easily be shown that for small y the function $\varphi(y)$ behaves as

$$\varphi(y) = \frac{16}{3\pi}y + \dots \tag{37}$$

so that

$$V(0) = \frac{4e^2}{3\pi^2\epsilon r} \tag{38}$$

The parameter $V(0)$ measures the Coulomb interaction between two electrons at the same point. In [22] this parameter is expressed in form $V(0) = e^2/(4\pi\epsilon b)$ and is evaluated from experimental values of the ionization energy and the electron affinity giving $b = 1.8 \times 10^{-10}$m for metallic platinum. This value of b can be used to obtain a rough estimate of the transverse size of the $Q1D$ system based on platinum compounds. The above value of b yields $r = 3.06 \times 10^{-10}$m. The value of r together with the interionic spacing ($a = 3.4 \times 10^{-10}$m) gives the ratio $r/a = 0.9$.

If we realize that

$$V(z) = \frac{e^2}{4\pi\epsilon}\int\int \frac{1}{(z^2 + |\mathbf{r}_\perp - \mathbf{r}'_\perp|^2)^{1/2}}\frac{\mathrm{d}^2r_\perp\,\mathrm{d}^2r'_\perp}{(\pi r^2)^2}, \tag{39}$$

we can derive the expansion of the function $\varphi(y)$ in the limit $y \to \infty$. Taking the expansion of the expression (39) we obtain:

$$\varphi(y) = \int\int\left(1 - \frac{|\mathbf{r}_\perp - \mathbf{r}'_\perp|^2}{2y^2r^2} + \dots\right)\frac{\mathrm{d}^2r_\perp\,\mathrm{d}^2r'_\perp}{(\pi r^2)^2} = 1 - \frac{1}{2y^2} + \dots \tag{40}$$

The function $\varphi(y)$ is shown in Fig. 2. We note that $\varphi(y)$ rapidly approaches 1 if the argument y proceeds to infinity.

IV. THE $Q1D$ FOURIER TRANSFORM OF POISSON'S EQUATION

Screening is one of the most important concepts in the treatment of systems containing electric charges. Charges, which are able, will move in response to an electric field (caused, e.g., by an external potential or by an impurity charge distribution). This charge motion will stabilize into a new distribution of charge around the electric field. The new induced charge distribution affords the screening potential which cancels the original electric field at large distances. The relation between the screening potential and the induced change in the charge distribution is set by Poisson's equation.

In this section we derive the $Q1D$ Fourier transform of Poisson's equation. The purpose of this treatment is to facilitate the study of the screening effect of the electron-electron and electron-ion interactions on the ion-ion interaction, to which the forth coming paper will be devoted.

Poisson's equation states:

$$\Delta V_s(\mathbf{r}) = -\frac{e^2}{\epsilon}\delta\varrho(\mathbf{r}) \tag{41}$$

where $V_s(\mathbf{r})$ is the screening potential and $\delta\varrho(\mathbf{r})$ is the induced change in the electron density which can be written in cylindrical coordinates $r_\perp$, φ, z as

$$\delta\varrho(r_\perp, \varphi, z) = \sum_{\substack{l,l'\\n,n'}} \varrho_{l,n;l',n'}(z)\,\psi^*_{l,n}(r_\perp, \varphi)\,\psi_{l',n'}(r_\perp, \varphi) \tag{42}$$

where $\varrho_{l,n;l',n'}(z)$ is the density matrix. The summation in (42) is performed over two sets of quantum numbers (l, n) and (l', n') which specify the state of the unperturbed electron system.

As in Sect. II we consider the case that only the ground state related to the transverse motion of the electrons is occupied and replace the ground state probability density by a constant value. Then we have:

$$\delta\varrho(r_\perp, \varphi, z) = \begin{cases} \dfrac{\delta\varrho(z)}{\pi r^2} & \text{for } r_\perp < r \\ 0 & \text{for } r_\perp > r \end{cases} \tag{43}$$

where $\delta\varrho(z)$ is the induced change of the $1D$ electron density.

If we employ that,the modified Bessel function of the second kind of the zeroth and argument $|q|\,|\mathbf{r}_\perp - \mathbf{r}'_\perp|$ is Green's function $G(\mathbf{r}_\perp, \mathbf{r}'_\perp, q)$ for the following differential equation [23]:

$$\frac{1}{r_\perp}\frac{\mathrm{d}}{\mathrm{d}r_\perp} r_\perp \frac{\mathrm{d}}{\mathrm{d}r_\perp} G(\mathbf{r}_\perp, \mathbf{r}'_\perp, q) - q^2 G(\mathbf{r}_\perp, \mathbf{r}'_\perp, q) = -\delta(\mathbf{r}_\perp - \mathbf{r}'_\perp) \tag{44}$$

where $\delta(x)$ is the Dirac delta function of argument x, and if we further carry out the $1D$ Fourier transform of Poisson's equation, we obtain the formal solution of equation (41) in the form:

$$V_s(\mathbf{r}_\perp, q) = \frac{e^2}{2\pi\epsilon}\delta\varrho(q)\int K_0(|q|\,|\mathbf{r}_\perp - \mathbf{r}'_\perp|)\frac{\mathrm{d}^2 r'_\perp}{\pi r^2} \tag{45}$$

where $V_s(\mathbf{r}_\perp, q)$ and $\delta\varrho(q)$ are the $1D$ Fourier transform of $V_s(\mathbf{r}_\perp, z)$ and $\delta\varrho(z)$, respectively. The integration is performed inside the circle of the radius r.

As we shall always be interested only in the interaction between the electrons in the ground state subband, we can average $V_s(\mathbf{r}_\perp, q)$ over the circle of the radius r:

$$V_s(q) = \int V_s(\mathbf{r}_\perp, q)\frac{\mathrm{d}^2 r}{\pi r^2} = v(q)\,\delta\varrho(q) \tag{46}$$

where again $v(q) = 2e^2\gamma(|q|\,r)/(\pi\epsilon)$.

Equation (46), which is the $Q1D$ Fourier transform of Poisson's equation, is of the same form as the usual $3D$ result except that the $3D$ Fourier transform of the Coulomb potential $e^2/(\epsilon q^2)$ is replaced by its $Q1D$ cunterpart $2e^2\gamma(|q|\,r)/(\pi\epsilon)$.

V. THE UNRENORMALIZED PHONON DISPERSION RELATION

In this section we further rearrange the ion part of the total Hamiltonian and obtain the unrenormalized phonon frequencies of the present model of the $Q1D$ electron-ion Coulomb a system. The treatment is largely based on the presentation given in [24].

Let the equilibrium position of the α-th ion be denoted by $Z_{\alpha 0} = \alpha_a$, where a is the interionic spacing. As the ions vibrate their actual position Z_α differs from the equilibrium position by the shift δZ_α: $Z_\alpha = Z_{\alpha 0} + \delta Z_\alpha$. Clearly, there is nothing which distinguishes the motion of the α-th ion from that of its neighbours. We can therefore write:

$$\delta Z_\alpha = \sum_k \frac{Q(k)}{(MN_i)^{1/2}} \mathrm{e}^{\mathrm{i}kZ_{\alpha 0}} \tag{47}$$

where $Q(k)$ are the N_i new coordinates, which describe the normal modes of osscillation of the ions about their equilibrium position and k is the wave vector from the first Brillouin zone defined by $-\pi/a < k \leq \pi/a$.

If the displacement of the ions from their equilibrium position is small, we can expand the ion-ion part of the Hamiltonian H_{ii} in a Taylor series. Retaining up to the quadratic terms in δZ_α we have:

$$H_{ii} = E_0 + \frac{1}{2L}\sum_{\alpha=1}^{N_i}\sum_{\beta=1}^{N_i}\sum_q q^2 w(q)(\delta Z_\alpha \delta Z_\beta - \delta Z_\alpha \delta Z_\alpha)\mathrm{e}^{\mathrm{i}q(Z_{\alpha 0} - Z_{\beta 0})} \tag{48}$$

where

$$E_0 = \frac{1}{2L}\sum_{\alpha=1}^{N_i}\sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_i}\sum_{q\neq 0} w(q)\mathrm{e}^{\mathrm{i}q(Z_{\alpha 0} - Z_{\beta 0})} \tag{49}$$

is the equilibrium position ion-ion interaction energy. Replacing δZ_α according to equation (47) and summing twice over the equilibrium position of the ions in equation (48) we obtain:

$$H_{ii} = E_0 + \frac{1}{2}\sum_k \Omega_{pl}^2(k)\,Q(-k)\,Q(k) \tag{50}$$

where $\Omega_{pl}^2(k)$ is given by

$$\Omega_{pl}^2(k) = \Omega_0^2(k) + \sum_{K_n\neq 0}[\Omega_0^2(k + K_n) - \Omega_0^2(K_n)] \tag{51}$$

where $\Omega_0^2(q) = q^2 w(q)/(aM)$ and K_n is the reciprocal lattice wave vector defined by $K_n = 2\pi n/a$, where n is an integer. It can easily be shown using the behaviour of the function $\gamma(x)$ at large values of the argument x (equation (33)) that the infinite series in (51) converges.

The kinetic part of the ion Hamiltonian can be rearranged with the aid of the following transformation:

$$P_\alpha = \sum_k \left(\frac{M}{N_i}\right)^{1/2} P(k)\,\mathrm{e}^{\mathrm{i}kZ_{\alpha 0}} \tag{52}$$

where $P(k)$ is the momentum conjugate to $Q(k)$.

In terms of the new coordinates the ion part of the Hamiltonian takes the form:

$$H_i = E_0 + \frac{1}{2}\sum_k [P(-k)P(k) + \Omega_{pl}^2(k)Q(-k)Q(k)]. \qquad (53)$$

The Hamiltonian (53) describes a harmonic-oscillator field decomposed into independent normal modes. Therefore, $\Omega_{pl}(k)$ can be identified with the unrenormalized phonon frequency of the $Q1D$ electron-ion Coulomb system for the wave vector k.

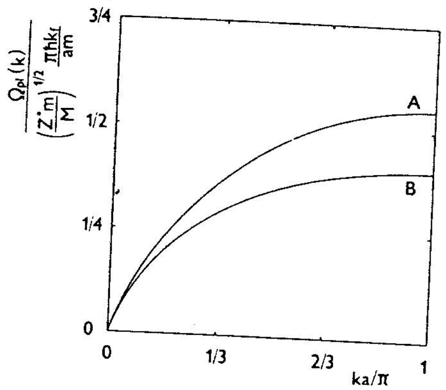

Fig. 3. The unrenormalized phonon frequency of the $Q1D$ electron-ion Coulomb system as the function of the wave vector (curve A is related to $r = 0.5$ a and curve B to $r = 0.9$a).

The unrenormalized phonon frequency as the function of the wave vector is shown in Fig. 3 for two different values of the parameter r. The phonon frequencies are plotted relative to $(Z^*m/M)^{1/2}\pi\hbar k_f/(am)$, which is the value of the $3D$ renormalized phonon frequency multiplied by $3^{1/2}$ and taken at π/a (i.e., at the $1D$ Debye wave vector). We have chosen $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$m, and $\epsilon_r = \epsilon/\epsilon_0 = 2.6$ (where ϵ_0 is the dielectric constant of vacuum). The curve labelled by A is related to $r = 0.5a$ and that labelled by B to $r = 0.9a$. The numerical values of the parameters Z^*, a, ϵ_r are taken from [25] and correspond to a platinum compound like KCP.

The expression (51) is of the same form as the sum rule of the squared unrenormalized phonon frequencies of the $3D$ system [24], in which the $3D$ Fourier transform of the ion-ion Coulomb interaction is replaced by its $Q1D$ counterpart. However, there is only a longitudinal mode of vibration in the present model of the $Q1D$ system, as the ions move only in one dimension. Moreover, the unrenormalized phonon frequency vanishes in the limit $k \to 0$, as it can be shown using equation (32). This behaviour is in contrast with that of the $3D$ system in which the longitudinal unrenormalized phonon frequency is

different from zero at $k = 0$. The reason for this difference is the "weakness" of the singularity of the $Q1D$ Fourier transform of the Coulomb potential at $k = 0$, which is only logarithmic.

VI. CONCLUSION

The $Q1D$ system, which consists of electrons confined to a cylindrical wire and interacting via the Coulomb interaction, was introduced by Lee and Spector [19]. We have included the ions into the model and have derived the form of the ion-ion and electron-ion matrices. As the electron-ion potential has been assumed to be the pure Coulomb potential, the interaction matrices obey the same relation as in the $3D$ model with the pure Coulomb potential.

The most common models of $1D$ systems, the Fröhlich model [2, 3] and the electron gas model [4], involve only one intrachain interaction, either the electron-phonon or the electron-electron interaction. In contrast with these models, the Hamiltonian of the present model involves both interactions. Moreover, the strengths of the interactions as well as unrenormalized phonon frequencies are not parametrised by constants but they are derived from first principles. Therefore, they propertly express the long-range nature of the Coulomb interaction. In most papers, only short-range interactions are considered, though there are some papers [15, 16, 26] which also treat the long-range nature of the electron-electron interaction.

The established parameters of the model have their clear physical meaning. However, a somewhat unusual parameter of the present model is probably the transverse size of the $Q1D$ system. In the original model [19], this parameter was established as the radius of the cylindrical wire the electrons are confined to. In the present model it is rather the effective transverse radius of the ions, which in turn determines the transverse size of the space the electrons can move in.

The reason for including the ions into the model is that we want to study the structural transition in the $Q1D$ system. The structural transition in low-dimensional systems originates from an anomaly in the electronic dielectric function at the weave vector $2k_f$, which in turn gives rise to an anomaly in the phonon spectrum.

Our forthcoming paper will deal with the study of the influence of the electrons on the phonon dispersion relation in the $Q1D$ electron-ion system described by the Hamiltonian which is derived in this paper.

ACKNOWLEDGEMENT

I thank Dr. S. Takács for some helpful comments on the manuscript.

REFERENCES

[1] Peierls, R. E.: *Qunatum Theory of Solids*. Oxford university, London, 1955.
[2] Berlinsky, A. J.: Rep. Prog. Phys. *42* (1979), 1243.
[3] Sham, L. J.: *Highly Conducting One-Dimensional Solids*, ed. Devreese, J. T., Evrard, R. P., van Doren, V. E., Plenum, New York, 1979.
[4] Sólyom, J.: Adv. Phys. *28* (1979), 201.
[5] Barišić, S.: J. Physique *44* (1983), 185.
[6] Schulz, H. J.: J. Phys. C *13* (1983), 6769.
[7] Botrić, S., Barišić, S.: J. Physique *45* (1984), 185.
[8] Suzumura, Y.: Prog. Theor. Phys. *61* (1979), 1.
[9] Okamoto, K.: Prog. Theor. Phys. *66* (1981), 852.
[10] Hubbard, J.: Proc. R. Soc. A *276* (1963), 238.
[11] Emery, V. J.: *Highly Conducting One-Dimensional Solids*, ed. Devreese, J. T., Evrard, R. P., van Doren, V. E., Plenum New York, 1979.
[12] Caron, L. G., Bourbonnais, C.: Phys. Rev. B *29* (1984), 4230.
[13] Baldea, J.: Phys. Scripta *31* (1985), 606.
[14] Voit, J., Schulz, H. J.: Mol. Cryst. Liquid Cryst. *119* (1985), 449.
[15] Kurihara, Y.: J. Phys. Soc. Jpn. *48* (1980), 1961.
[16] Nakane, Y., Takada, S.: J. Phys. Soc. Jpn. *54* (1985), 977.
[17] Abramowitz, M., Stegun, I. A.: *Handbook of Mathematical Functions*. Dover, New York, 1964.
[18] Ryžik, I. M., Gradštein, I. C.: *Tablicy Integralov, Sum, Radov i Proizvedenij*, Fizmatgiz, Moskva, 1962.
[19] Lee, J., Spector, H. N.: J. Appl. Phys. *57* (1985), 366.
[20] Maksimov, E. G., Khomskii, D. J.: *High-Temperature Super conductivity*. ed. Ginzburg, V. L., Kirzhnits, D. A., Consultants, New York, 1982.
[21] Dzialošinskij, I. E., Kats, E. J.: Ž. Eksp. Teor. Fiz. *55* (1968), 338.
[22] Davis, D., Gutfreund H., Little, W. A.: Phys. Rev. B *13* (1976), 4766.
[23] Jackson, J. D.: *Classical Electrodynamics*. Wiley, New York, 1962.
[24] Pines, D.: *Elementary Excitations in Solids*. W. A. Benjamin, New York, 1963.
[25] Gutfreund, H., Little, W. A.: *Highly Conducting One-Dimensional Solids*. ed. Devreese, J. T., Evrard, R. P., van Doren, V. E., Plenum, New York, 1979.
[26] Barišić, S., Tutić, F.: J. Phys. C *19* (1986), 6303.

Received May 28th, 1987
Revised version received July 23rd, 1987
Accepted for publication August 3rd, 1987

МОДЕЛЬ КВАЗИОДНОМЕРНОЙ ЭЛЕКТРОН—ИОННОЙ КУЛОНОВСКОЙ СИСТЕМЫ И. ОБЩАЯ ФОРМУЛИРОВКА

На основе первых принципов в работе выведена функция Гамильтона квазиодномерной системы. Предполагается, что электроны и ионы системы взаимодействуют только посредством кулоновского взаимодействия. Обнаружено, что матрицы взаимодействия имеют логарифмическую рассходимость в пределе нулевого волнового вектора. Она является

послествием дальнодействующего характера кулоновского потенциала. Вследствие того, что рассходимость имеет логарифмический характер, неперенормированная частота фононов равнается нулю когда волновый вектор стремится внулю. В работе тоже детально рассмотривается зависимость преобразования фурье кулоновского потенциала от поперечного размера системы. Далее выведено квазиодномерное преобразование фурье уравнения Пуассона.

Влияние электрон-ионного и электрон-электронного взаимодействия на частоты фононов будет рассматриваться в следующей статье.