MODEL OF THE QUASI-ONE-DIMENSIONAL ELECTRON-ION COULOMB SYSTEM III. THERMAL PROPERTIES

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We present a numerical calculation of the mean-field temperature of the Peierls transition whose presence in the quasi-one-dimensional system is proved in Part II. We also settle restrictions on the temperature that must be obeyed for the description of the properties of the quasi-one-dimensional system of electrons and ions with the Hamiltonian derived in Part I to be correct. From the obtained values of the characteristic temperatures, implications concerning the phase state the system condenses in are drawn.

I. INTRODUCTION

Properties of 1D systems have been studied mainly with the help of the mean-field theory in which effects of fluctuations are disregarded. The mean-field theory of the Peierls transition in 1D metals was originally proposed by Fröhlich [1] and Kuper [2]. Later it was elaborated by many authors [3—5]. The mean-field calculation predicts that the initial high-temperature lattice turns out to be unstable at the Peierls transition temperature:

$$T_{P} = \frac{\gamma \hbar^{2} k_{L}^{2}}{\pi m k_{B}} e^{-1/\lambda}$$

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where λ is the dimensionless electron-phonon interaction parameter of the Fröhlich model given by $\frac{2g^2m}{(2)}$

$$\lambda = \frac{2g^2 m}{\hbar \Omega_0(2k_f) \pi \hbar^2 k_f} \tag{2}$$

and $\ln \gamma = C = 0.5772...$ is the Euler constant. All the other parameters are defined in Part II (foregoing paper in this issue).

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parameter λ to which all the phonons contribute [6, 7]: electrons, the Peierls transition temperature is determined by the dimensionless In more complex 1D systems, in which several phonon bands couple to the

$$\lambda_{n} = \sum_{n} \lambda_{n}, \qquad \lambda_{n} = \frac{2g_{n}^{2}m}{\hbar \Omega_{0,n}(2k_{f}) \pi \hbar^{2}kf}.$$
 (3)

Thus, the greater λ_n is, the more strongly the phonons in question take part in

3D oscillations of phonons of a single chain also enable the true phase transition degree of the interchain coupling is sufficient to bring the actual transition and quantum fluctuations shift the phase transition to zero temperature temperature close to the mean-field value [16]. It must be mentioned here that sensitive function of the interchain coupling and as it is known now, a small $T \lesssim T_p/4$. The factor 1/4 is somewhat arbitrary. As a matter of fact, it is a Q1D systems, according to the estimate of Lee et al. [15] at the temperature behaviour of the system. Therefore, a true phase transition is observed in the range order in the transverse direction resulting in a crossover to the 3Dfluctuations. Thus, the interchain coupling enables the development of longwho showed that the interchain coupling partially suppresses the effects of a little complicated by the fact that 1D systems are not supposed to exhibit phase [10-14]. A way out of this dilemma was first proposed by Lee et al. [15] transition at nonzero temperature [8, 9]. Namely it is well known that thermal However, the application of the 1D mean-field theory to real Q1D solids is

numerically compute the transition temperature of the Q1D electron-ion Coucalculations. In this paper we extend the existing calculations of the transition towards the Peierls transition. lomb system which, as shown in the foregoing paper, exhibits an instability temperature to account for the effect of periodicity of the lattice. Further, we interpreting experiments and therefore it seems worthwhile to improve such Despite their limitations, results of the mean-field theory have been useful in

deriving the model Hamiltonian of the Q1D electron-ion system. We use a of the harmonic approximation. This approximation was used in Part I [18] for temperature which must be obeyed for the model Hamiltonian to be correct. formal expression of the anharmonic terms to obtain a restriction on the formulae from the thermodynamics of the phonon system to discuss the validity Besides the transition temperature calculation, we give a few fundamental

thermodynamics is applied to the present model of the ion system The arrangement of the paper is as follows: in Sect. II the elementary

exhibits an instability of the Peierls type. In Sect. III we calculate the temperature at which the Q1D electron-ion system

II. THE THERMODYNAMICS OF THE ION SYSTEM

a system of independent harmonic oscillators. The calculation of the therroute followed for the harmonic oscillator [8]. modynamic quantities of the ion system then proceeds along the well-known ground of negative charge can be described in the harmonic approximation as As shown in I, the 1D ion Coulomb system immersed in a uniform back-

The Helmholtz free energy of the ion system is

$$F_{i} = E_{0} + k_{B} T \sum_{k} \ln \left\{ 2 \operatorname{sh} \left[\frac{\hbar \Omega_{pl}(k)}{2k_{B} T} \right] \right\}. \tag{4}$$

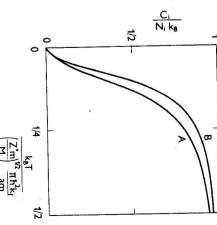
the energy Knowing the free energy we can obtain the thermodynamic quantities as, e.g.

$$E_{i} = F_{i} - T \frac{\partial F_{i}}{\partial T} = E_{0} + \frac{1}{2} \sum_{k} \hbar \Omega_{pl}(k) \operatorname{cth} \left[\frac{\hbar \Omega_{pl}(k)}{2k_{B}T} \right]$$
 (5)

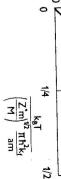
the specific heat

$$C_{i} = \frac{\partial E_{i}}{\partial T} = k_{B} \sum_{k} \left\{ \frac{\hbar \Omega_{pl}(k)}{2k_{B} T \operatorname{sh} \left[\frac{\hbar \Omega_{pl}(k)}{2k_{B} T} \right]} \right\}$$
 (6)

etc. The plot of the specific heat as a function of the temperature is shown in I and II, throughout this paper the other parameters take the following values Fig. 1 for two values of the parameter r, namely, r = 0.5a and r = 0.9a. As in $Z^* = 5/3$, $a = 3.4 \times 10^{-10}$ m, $\epsilon_r = 2.6$. We emphasize once more that all the



charge (curve A is related to r = 0.5a and curimmersed in a uniform background of negative Fig. 1. The specific heat of the 1D ion system ve B to r = 0.9a)



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thermodynamic quantities obtained in this section express the properties of the 1D ion system immersed in a uniform background of negative charge.

Using the expansion of the hyperbolic functions at a small value of the argument $(\hbar\Omega_{pl}(k) \leqslant k_BT)$, we get in the high temperature limit

$$F_i = E_0 + k_B T \sum_k \ln \left[\frac{\hbar \Omega_{pl}(k)}{k_B T} \right] + \dots$$
 (7)

$$E_i = E_0 + N_i k_B T + \dots$$
 (8)

$$C_i = N_i k_B + \dots$$

Fig. 1 gives an idea about the values of the temperature that can be regarded high because of $(Z^*m/M)^{1/2}\pi\hbar^2k_f/(amk_B) = 1.36 \times 10^3$ K for our choice of the parameters Z^* , a, \in , and $M = 3.26 \times 10^{-25}$ kg (corresponding to the mass of the platinum atom). We remind that the numerical values of the parameters correspond to a platinum compound like KCP (see the foregoing paper).

So far, our attention in the treatment of the ion vibrations has been confined only to the harmonic term in the expansion of the ion-ion interaction potential, i.e., to the term which is quadratic in the displacements of the ions from their equilibrium positions. However, at high temperatures the effects of the anharmonic terms (cubic, biquadratic etc.) in the ion displacements may become important. We now estimate the temperature at which the anharmonic terms are to be taken into account.

Landau and Lifshitz [8] showed that the first correction of the free energy (equation (7)) due to the anharmonic terms has the form $F_{l,outh} = AT^2$. This correction is valid at high temperatures, at which quantum effects are unimportant because the correction was obtained by methods of classical statistical physics. As Landau and Lifshitz [8] emphasized the expansion in question is essentially an expansion in the power series of the parameter $N_i k_B T_i / |E_0|$ and not $k_B T / \hbar \Omega_{pi}(k)$, which is large in this case. Hence we conclude that the anharmonic terms do not have to be considered as far as

$$T \leqslant T_i = |\epsilon_0|/k_B \tag{10}$$

where ε_0 is the ion-ion equilibrium position energy per ion. It can be expressed in the form

$$\mathcal{E}_{0} = \frac{E_{0}}{N_{i}} = \frac{1}{2N_{i}L} \sum_{\alpha=1}^{N_{i}} \sum_{\substack{\beta=1 \ \beta \neq \alpha}}^{N_{i}} \sum_{\substack{q \neq 0}} w(q) e^{iq(Z_{\alpha 0} - Z_{\beta 0})} = \\
= -\frac{Z^{*2}e^{2}}{\pi \in aN_{i}} \left[\sum_{\substack{q \neq 0}} \gamma(|q|r) - N_{i} \sum_{\substack{K_{n} \neq 0}} \gamma(|K_{n}|r) \right] = -\frac{Z^{*2}e^{2}}{\pi \in a} \left[\frac{2a}{3\pi r} - \sum_{\substack{K_{n} \neq 0}} \gamma(|K_{n}|r) \right].$$
(11)

The plot of ε_0 as a function of the transverse radius of the ions is shown in Fig. 2. We note that $Z^{*2}e^2/(\pi \epsilon ak_B) = 2.1 \times 10^5$ K.

There is still another possible interpretation of equation (10), namely, as a stability criterion of the 1D ion system against melting. According to the idea of L in demann [19] (see e.q. [20]), a solid melts because the vibrations of the ions about their equilibrium positions become too large. In a 3D system, the ion vibrations are considered to be large when the mean-square amplitude of vibrations is comparable to the square of the interionic spacing. This criterion of large vibrations is not applicable to a 1D ion system. The reason for this is that the calculation of the 1D mean-square amplitude of vibrations as well as that energy of vibrations of the 1D fluctuation quantities yields a divergent result at a small wave vector. The 1D vibrations of the ions can be regarded large when the energy of vibrations is comparable with the ion-ion equilibrium position energy. Since at high temperatures the energy of vibrations is $N_i k_B T$ (equation (8)) and the ion-ion equilibrium position energy is $N_i k_B$, we now obtain the condition (10) as a stability criterion against melting. Thus, the melting temperature is

$$T_{m} = \gamma_{m} T_{i}, \tag{12}$$

where γ_m is a dimensionless parameter which may depend on the ion size.

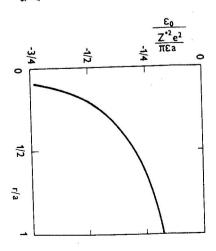


Fig. 2. The ion-ion equilibrium position energy per an ion as a function of the transverse radius of the ions.

The obtained melting temperature expresses only properties of the 1D ion system. It may happen that the temperature of the chemical decomposition of the surrounding insulating media is lower than the 1D melting temperature given by equation (12). In such a case, T_m means the decomposition temperature. Because of this, the temperature T_m obtained from equation (12) can be regarded as the upper limit settled on the value of the melting temperature.

Anyway, T_i gives the restriction on the temperature because the ion part of the total Hamiltonian correctly describes a 1D ion system only as far as the temperature is much lower than T_i . Another restriction on the temperature was given in Part I. It was shown that the electron as well as the electron-ion parts of the Hamiltonian are correct as far as

$$T \ll T_e = \frac{\hbar^2}{2mr^2k_B}. (13)$$

The condition (13) ensures that only the ground state subband related to the transverse motion of the electrons is occupied.

At this point, it is necessary to point out that the impossibility of a phase transition in a 1D system due to thermal fluctuations was determined on the basis of thermodynamic considerations. The thermodynamics predicts that a long-range order which is always settled at the phase transition, cannot exist in the equilibrium state. However, in thermodynamics the question of equilibration time is not considered and the destruction of a long-range order is determined even in the case when the probability for it is extremely small. It is clear that as far as the temperature obeyes the condition (13) the appearence of the fluctuations in question is highly improbable. And if also the actual transition temperature of the Q1D system obeyes the condition (13), it can be determined on the basis of the mean-field calculation. In the opposite case, it can differ from the mean-field result.

III. THE TRANSITION TEMPERATURE

As indicated in the foregoing paper, the transition temperature T_p is the solution of equation

$$\Omega_{ph, T_p}^2(2k_f) = 0,$$
 (14)

where the squared renormalized phonon frequency at the wave vector $2k_f$ and at the temperature T is defined by

$$\Omega_{ph, T}^{2}(2k_{f}) = \Omega_{0}^{2}(2k_{f}) + \sum_{K_{n} \neq 0} \left[\Omega_{0}^{2}(2k_{f} + K_{n}) - \Omega_{0}^{2}(K_{n}) \right] - \\
- \Omega_{a}^{2}(2k_{f}) - \sum_{K_{n} \neq 0} \left[\Omega_{a}^{2}(2k_{f} + K_{n}) - \Omega_{a}^{2}(K_{n}) \right] + \\
+ \frac{\Omega_{a}^{2}(2k_{f})}{\epsilon_{T}(2k_{f}, 0)} + \sum_{K_{n} \neq 0} \left[\frac{\Omega_{a}^{2}(2k_{f} + K_{n})}{\epsilon_{T}(2k_{f} + K_{n}, 0)} - \frac{\Omega_{a}^{2}(K_{n})}{\epsilon_{T}(K_{n}, 0)} \right].$$
(15)

The 1D dielectric function $\epsilon_T(2k_f, 0)$ is logarithmically singular as $T \to 0$. Therefore, $\Omega_s^2(2k_f)/\epsilon_T(2k_f, 0)$ does not contribute to the squared renormalized

phonon frequency at zero temperature. Being summed up the remaining terms give the negative value of the squared renormalized phonon frequency as the $Q \mid D$ electron-ion system is supposed to undergo the structural phase transition. With rising temperature, $\Omega_{\sigma}^2(2k_f)/\epsilon_T(2k_f,0)$ gradually increases and at the transition temperature, it cancels the total negative contribution of the remaining sition temperature it follows that the main point of the transition temperature calculation is the determination of the temperature dependence of the 1D dielectric function at $2k_f$. It was shown in II that in the RPA approximation, the 1D dielectric function at $2k_f$ is given by

$$\epsilon_T(2k_f, 0) = 1 - v(2k_f) \Lambda_T(2k_f, 0),$$
(16)

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$$A_{r}(2k_{j}, 0) = -\frac{m}{2\pi\hbar^{2}k_{f}} \int_{-\infty}^{\infty} \left[\frac{f(q-k_{j}) - f(q+k_{j})}{q} \right] dq.$$
 (17)

It is not possible to calculate the integral in the expression (17) analytically. To obtain an analytical though very approximative expression of $\Lambda_T(2k_f, 0)$, the integral is usually estimated in the following way [21]. First, the electronic dispersion relation is linearized, i.e., $E(q-k_f) - \hbar^2 k_f^2/(2m) \simeq -\hbar^2 k_f q/m$ and $E(q+k_f) - \hbar^2 k_f^2/(2m) \simeq \hbar^2 k_f q/m$. It is a reasonable approximation only in the neighbourhood of q=0. Then, it is necessary to introduce the bandwidth cut-off to avoid the divergence of the integral caused by the linearization of the electronic dispersion relation. So the wave vector q is supposed to lie between $-k_f/2 \le q \le k_f/2$. The choice of $k_f/2$ as a bandwidth cut-off ensures that the spectra. Various aspects of the linearization of the electronic spectrum and the problem of the bandwidth cut-off are discussed, e.g., in [10, 22, 23].

Thus, $\Lambda_T(2k_f, 0)$ takes the form

$$A_T(2k_f, 0) = -\frac{m}{\pi \hbar^2 k_f} \int_0^{4\pi k_B T} \frac{\text{th}(y)}{y} \, \mathrm{d}y.$$
 (18)

As fat as $T \ll \hbar^2 k_f^2/(4mk_B)$ (= 1.31 × 10⁴K for our choice of the parameters Z^* and a), the calculations can proceed along the route known from the theory of superconductivity [24]:

$$A_{T}(2k_{f}, 0) = -\frac{m}{\pi \hbar^{2} k_{f}} \ln \left(\frac{\gamma \hbar^{2} k_{f}^{2}}{\pi m k_{B} T} \right). \tag{19}$$

Now, the equation (14) can be rewritten in the form

$$T_{P} = \frac{\gamma \hbar^{2} k_{L}^{2}}{\pi m k_{B}} \exp\left(-1/\lambda_{T_{P}}\right), \tag{20}$$

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electron-ion system λ_T at the temperature T is given by where the dimensionless electron-phonon interaction parameter of the Q1D

$$\lambda_{T} = \frac{mv(2k_{f})}{\pi k_{f} \hbar^{2} \Omega_{a}^{2}(2k_{f})} \left[\Omega_{a}^{-2}(2k_{f}) + \left\{ \Omega_{0}^{2}(2k_{f}) + \sum_{K_{n} \neq 0} \left[\Omega_{0}^{2}(2k_{f} + K_{n}) - \Omega_{0}^{2}(K_{n}) \right] - \Omega_{a}^{2}(2k_{f}) - \sum_{K_{n} \neq 0} \left[\Omega_{a}^{2}(2k_{f} + K_{n}) - \Omega_{a}^{2}(K_{n}) \right] + \right.$$

$$\left. + \sum_{K_{n} \neq 0} \left[\frac{\Omega_{a}^{2}(2k_{f} + K_{n})}{\epsilon_{T}(2k_{f} + K_{n}, 0)} - \frac{\Omega_{a}^{2}(K_{n})}{\epsilon_{T}(K_{n}, 0)} \right] \right\}^{-1} \right\}^{-1}.$$

$$(21)$$

dimensionless electron-phonon interaction parameter is independent of the temperature and has the form In the jellium approximation, when all aspects of periodicity are neglected, the

$$\lambda = \frac{m}{\pi \hbar^2 k_f} \left[\frac{u^2(2k_f)}{w(2k_f)} - v(2k_f) \right]. \tag{22}$$

and Takada [25]. expresses the transition temperature of the Q1D electron-ion system in the jellium approximation. It corresponds to the formula obtained by Nakane The expression (20) together with λ given by equation (22) approximately

In the present model, $\Omega_a^2(2k_f) = \Omega_0^2(2k_f)$ and equation (21) reduces to

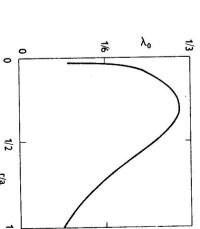
$$\lambda_{T} = -\frac{mv(2k_{f})}{\pi\hbar^{2}k_{f}} \left\{ 1 + \frac{\Omega_{0}^{2}(2k_{f})}{\sum_{K_{n} \neq 0} \left[\frac{\Omega_{0}^{2}(2k_{f} + K_{n})}{\epsilon_{T}(2k_{f} + K_{n}, 0)} - \frac{\Omega_{0}^{2}(K_{n})}{\epsilon_{T}(K_{n}, 0)} \right] \right\}^{-1}.$$
 (23)

approximative formula for the transition temperature of the present model of phonon interaction parameter at zero temperature. Then, we have the final the Q1D electron-ion Coulomb system: Numerical computations prove that λ_T slightly varies with the temperature. Therefore, in equation (20) λ_T can be replaced by λ_0 , the dimensionless electron-

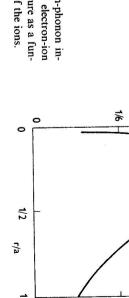
$$T_{P,0} = \frac{\gamma \hbar^2 k_f^2}{\pi m k_B} \exp\left(-1/\lambda_0\right). \tag{24}$$

electron-phonon parameter of the Fröhlich model only on the strength of the the foregoing paper, the transition in the Fröhlich model appears to be only a transition temperature in the Fröhlich model. However, as it is emphasized in phonon frequencies. It manifests itself in the dependence of the dimensionless result of the influence of the electron-phonon interaction on the unrenormalized The obtained expression (24) is of the same form as the expression (1) for the

> model of the Q1D system appears to be a result of the influence of both the electron-phonon interaction. On the other hand, the transition in the present electron-ion interaction and the electron-electron interaction. Because of this, electron-phonon parameter of the present model of the Q1D system (equation the strengths of both interactions enter in the expression for the dimensionless



teraction parameter of the Q1D electron-ion Coulomb system at zero temperature as a fun-Fig. 3. The dimensionless electron-phonon inction of the transverse radius of the ions.



of the ions. The numerical values of the transition temperature for some values equation (14), $T_{P,0}$'s are obtained from equation (24), T_i 's and T_i 's from equacharacteristic temperatures of the present model of the Q1D electron-ion Couof the transverse radius of the ions are presented in Table I, where also the other tions (10) and (13), respectively. The parameters Z^* , a, ϵ , have their values lomb system are summarized. Namely, T_p 's are the numerical solutions of itself in the dependence of the transition temperature on the transverse radius the ions, which is shown in Fig. 3. Of course, this sensitivity strongly manifests mentioned earlier. Of particular note is the extreme sensitivity of λ_0 to the transverse radius of

estimation of the integral in equation (17). The transition temperature ranges ratio $T_P/T_{P,\,0}$. The difference between T_P and $T_{P,\,0}$ is caused by the incorrect the melting temperature of the whole system. As the transition temperature reaches such high values it must be compared with from the value about zero (for r = a) to the value over 3000 K (for r = 0.3a). transition temperature $T_{P,0}$. The higher the temperature is, the smaller is the The numerically computed transition temperature T_p is higher than the

suitable technique to treat the Hamiltonian as it was done for the Fröhlich far as $T > T_p$. At T_p it undergoes a structural phase transition of the Peierls type. To describe the behaviour of the system below T_p it is necessary to develop a Evidently, when $T_p < T_m$, the Q1D electron-ion system is in a metalic state as

model by Lee et al. [26] or for the Q1D electron-ion model in the jellium approximation by Nakane and Takada [25]. When $T_p > T_m$, the system is in the structural state of the Peierls type and at T_m it is destroyed by melting or by chemical decomposition. For example, let us suppose that the melting temperature is in the region $T_m \approx 1500 \div 2000 \,\mathrm{K}$. Such values of T_m can be obtained from equation (12) with $\gamma_m \approx 1/20$ for $r \approx 0.8a \div a$, for the other values of r, we consider that the system "melts" at T_m because of the chemical decomposition of the surrounding organic media. Comparing T_p with T_m we conclude that the Q1D system, which can be described by the present model with the parameters Z^* , a, ϵ , given above and $r \lesssim 0.5a$, is in the state of the Peierls type below T_m .

The characteristic temperatures of the Q1D electron-ion Coulomb system for some values of the transverse radius of the ions

3.83 × 10 ³	3.69×10^{4}	1.89×10^{-1}	7.53×10^{-1}	1.0
4.72×10^{3}	4.02×10^4	2.81×10^{0}	1.12×10^{1}	0.9
5.98×10^{3}	4.42×10^4	2.25×10^{1}	8.89×10^{1}	0.8
7.81×10^{3}	4.90×10^4	1.06×10^{2}	3.80×10^{2}	0.7
1.06 × 10°	5.49×10^4	3.22×10^{2}	9.64×10^{2}	0.6
1.53 × 10°	6.24×10^4	6.76×10^{2}	2.06×10^{3}	0.5
2.39×10°	7.24×10^4	1.04×10^{3}	2.87×10^{3}	0.4
4.25 × 10°	8.62×10^4	1.20×10^{3}	3.10×10^{3}	0.3
9.56 × 10"	1.08 × 10°	1.03×10^{3}	2.71×10^{3}	0.2
3.83×10^5	1.51×10^5	5.75×10^2	1.70×10^{3}	0.1
7, [K]	<i>T,</i> [K]	$T_{P,0}$ [K]	T_{ρ} [K]	r/a
				- 1

IV. CONCLUSION

In the series of papers we have developed the microscopic model of the Q1D system of the electrons and ions interacting through the pure Coulomb interaction. To summarize the main results, in Part I the Hamiltonian of the proposed model was derived from first principles. Determining the squared renormalized phonon frequencies we showed in Part II that the Q1D system with the chosen parameters exhibits an instability towards the Peierls transition. Finally, in this paper we calculated the transition temperature.

The main advantage of the present model of the Q1D system over other 1D models lies in the fact that it was derived from first principles. Therefore, its Hamiltonian properly includes all the intrachain interparticle interactions, namely, the ion-ion, electron-ion and electron-electron interactions. Though we have supposed that the particles of a single chain interact only according to the

Coulomb law, our method of deriving the Hamiltonian allows the subsequent inclusion of the non-Coulombic short-range part of the intrachain interparticle interaction or any type of the interchain interaction. We emphasize once more that in Part II we correctly showed the reason of the structural transition of the Peierls type. Namely, this transition is not caused only by the electron-ion interaction alone, as it is usually explained on the basis of the Fröhlich model, but by the effect of the mutual interplay between the electron-ion and electron-electron interactions on the unrenormalized phonon frequencies.

In addition to fundamental physical constants, the model includes five other eligible parameters, namely, M (the ion mass), Z^* (the effective valence), a (the eligible parameters, namely, M (the ion mass), Z^* (the effective valence), a (the interionic spacing), ϵ_r (the relative dielectric constant of the surrounding organic media), and r (the transverse radius of the ions). With the exception of the parameter r, all the other parameters were chosen in the numerical calculations to correspond to a platinum compound like KCP. As the exact value of the parameter r is not known to us (it was only estimated very roughly in Part I), the most important quantities were usually computed for a whole region of its values ($r \approx 0 + a$). But this parameter strongly influences the implications drawn from the model. For example, the transition temperature is very sensitive to it. Therefore, it is necessary to know its exact value in order to predict the transition temperature of a real Q1D system. On the other hand, it is possible to determine the parameter r from the known value of the transition temperature and then after a further development of the model, to compare the calculated quantities with experimental data.

We also point out that so far we have made numerical calculations only with the values of the parameters given above. Therefore, it is possible that a Q1D electron-ion system with some other values of the parameters Z^* , a, ϵ , and r does not exhibit the Peierls transition at all. We also note that we studied an ideal, defect-free Q1D system and a small amount of impurities can suppress the Peierls transition. A better approximation, which goes beyond the RPA, may also improve the obtained results. There are many other possibilities for the improvement of the model in order that it may provide a better picture of real C1D systems.

Notwithstanding all this, the present model is interesting in its own right, apart from its possible relevance to real systems, as it exhibits typical 1D effects. It is hoped that further study will lead to the description of its behaviour below the transition temperature.

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ЭЛЕКТРОН-ИОННОЙ КУЛОНОВСКОЙ СИСТЕМЫ МОДЕЛЬ КВАЗИОДНОМЕРНОЙ **III. ТЕПЛОТНЫЕ СВОЙСТВА**

мильтонияном выведеным в І-ой части являлось правильным. Из полученных величин хараквыполнены, чтобы описание свойств квазиодномерной системы электронов и ионов с гасистема конденсирует теристических температур выведены следствия касающиеся фазового состояния, в котором но в II-ой части. Мы тоже накладываем ограничения на температуру, которые должны быть в приближении среднего поля, появление которого в квазиодномерной системе подтвержден В работе представляем нумерические вычисления температуры пайерлсовского перехода