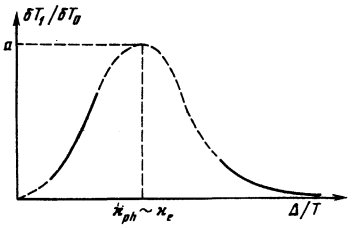

FIG. 2. Dependence of $\delta T_1/\delta T_0$ on Δ/T; $a = \frac{1}{10}\left(\frac{\varkappa_e^n}{\varkappa_{ph}^n}\Big|_{T=\Delta}\right)^{1/3}$.

tional Kapitza jump in the case of a superconductor with finite thickness d assuming identical boundary conditions on both boundaries

$$\delta T_1(d)/\delta T_1(\infty) = 2\mathrm{th}\,(d/2\lambda). \qquad (31)$$

The coefficient 2 is connected with the fact that we have calculated the additional jump on both boundaries. With decreasing sample thickness, the additional jump tends to zero. To observe this phenomenon it is necessary to have samples with thickness $d<\lambda$.

In order of magnitude, λ is equal to $L_s^{>} \sim e^{\Delta/T} l_{im}^{1/2}$ (this can be verified by recognizing that the electron-phonon and phonon-electron relaxation times are proportional to the same electron-phonon interaction constant and differ only in the final state densities), and can vary in a wide range, depending on the purity of the sample (i.e., on l_{im}) and on the temperature. For example, at $l_{im}=10^{-6}$ cm and $\Delta/T=2$, $l_{>}=10^{-5}$ cm we have $\lambda \approx 10^{-3}$ cm, while at $l_{im}=10^{-2}$ cm and $\Delta/T=5$ we have $\lambda \approx 1$ cm.

The sign of the additional jump and its order of magnitude can be reconciled with the experimentally observed values. For a more detailed comparison of experiment with theory, however, measurements in a larger temperature interval are needed.

A phenomenon similar to that considered above can arise also in He II, where there is likewise a hierarchy of phonon and roton relaxation lengths,[2] and according to estimates[2,11] the energy is transported through the boundary, in the region $T \gtrsim 1$ K, the rotons make the main contribution to all the thermodynamic functions and it is precisely they which transport the energy. This should produce in He II a relaxation region similar to that considered in the superconductor. We shall not, however, discuss this possibility in greater detail.

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Effect of electron interaction on the Peierls instability

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The dependence of the energy of the ground state of a one-dimensional metal on the amplitude of a periodic deformation is considered in the Hubbard model for different values of the interelectron-interaction parameter. It is shown that a Mott one-dimensional dielectric is unstable to the Peierls deformation at all values of the interaction parameter. Relations are obtained between the responses to the perturbations with wave numbers $Q = 2k_F$ and $4k_F$ in the limiting case of strong and weak electron interaction.

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INTRODUCTION

The instability of a one-dimensional metal to lattice deformation leads to the onset of a Peierls-Fröhlich state.[1-5] The investigation of various characteristics of this state is of interest because of the advent of new quasi-one-dimensional conductors.[3-8]

The conclusion that a one-dimensional metal is unstable to lattice deformation was deduced by Peierls on

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the basis of a calculation in the noninteracting-electron approximation, in which the period of the deformation is $\lambda_F = \pi/k_F$, where k_F is the Fermi momentum. The influence of the interaction of the electrons on the appearance of instability has not been sufficiently well investigated. At the same time, this question is important, since the interelectron distance in a one-dimensional system also gives rise to a transition into a dielectric state, namely the Mott transition.[9-14] An investigation of the system in the very-strong-interaction limit points to the appearance of instability to deformation, with a period $\lambda_F/2$.[15,16]

Methods based on the single-determinant approximation for the wave function are insufficient for the description of a one-dimensional system of interacting electrons.[9-16] The need for using more complicated approximations is the cause of the main difficulty encountered in the study of the role of interelectron interaction in a one-dimensional metal. In the present paper we describe a multielectron system by a previously described[17] variational approach which makes it possible to take correlations effect into account. We consider on the basis of this approach the influence of the electron interaction on the Peierls instability in an infinite chain of identical centers, containing ρ electrons per center. We consider in greatest detail the case $\rho = 1$, when the one-dimensional system is a Mott dielectric. For the case $\rho < 1$, we discuss the role of deformations with periods λ_F and $\lambda_F/2$ at different values of the interaction parameter. The analysis consists of a study of the dependence of the system ground-state energy on the amplitude of the periodic deformation, i.e., in the approximation of a frozen-in core. The results are used to discuss the experimental data on the Peierls instability of a number of quasi-one-dimensional systems based on TCNQ.[8,18]

1. LATTICE DEFORMATION IN A LINEAR HUBBARD CHAIN

To describe the conduction electrons we use the one-dimensional Hubbard Hamiltonian

$$\mathcal{H} = -\sum_{\substack{m=1\\ \sigma}}^{N} \beta_m (c_{m\sigma}^{+} c_{m+1,\sigma} + c_{m+1,\sigma}^{+} c_{m\sigma}) + \gamma \sum_{m=1}^{N} (c_{m\uparrow}^{+} c_{m\uparrow} c_{m\downarrow}^{+} c_{m\downarrow}), \tag{1}$$

where $\beta_m > 0$, $c_{m\sigma}^{+}$ is the operator for the creation of an electron with spin σ at the site m, and N is the number of sites.

We assume that in the undeformed chain all the resonant integrals are identical: $\beta_m = \beta$. In this case the Hamiltonian (1) is characterized by a single parameter $U = \gamma/\beta$. Displacement of the mth atom of the chain as a result of periodic deformation will be represented in the form

$$x_m = \Delta r_m/a = x \cos(Qma + \varphi), \tag{2}$$

where a is the constant of the undeformed lattice, x is the dimensional amplitude of the deformation wave, and φ is its phase. The appearance of displacements of the atoms leads to a change in the bodies of the resonant integrals, which are functions of the interatomic distances. In the simplest case of a half-filled band the Peierls deformation reduces to a doubling of the period of the lattice, i.e.,

$$\beta_m = \beta[1 + (-1)^m \Delta]. \tag{3}$$

At small displacements, the parameter Δ is linearly connected with the deformation amplitude ax:

$$\Delta = ax\beta'/\beta, \tag{4}$$

where β' is the derivative of β with respect to the interatomic distance.

We reduce the problem of investigating the instability of a one-dimensional metal, following Peierls, to the study of the dependence of the energy of the ground state on the parameter Δ. The lattice contribution will be set equal to $M(\omega ax)^2/2$, where M is the mass of the ion, and ω is the "bare" frequency of the acoustic oscillation with wave number $Q = 2k_F$. Thus, to solve our problem we must find that value of Δ which minimizes the expression

$$\varepsilon_t(\Delta) = \varepsilon(\Delta) + \Delta^2/2b, \tag{5}$$

where the symbol $\varepsilon(\Delta)$ stands for the specific electron energy in units of β, and $b = (\beta')^2/\beta M\omega^2$ is a dimensionless parameter that characterizes the magnitude of the electron-phonon interaction.

Let us list briefly some of the results concerning the Peierls instability of a system with Hamiltonian (1) at $\beta_m = \beta$. At $U = 0$, the ground state of the system is described by a Slater determinant Ψ_0 made up of Bloch functions corresponding to the operators that diagonalize the kinetic energy in (1), i.e.,

$$\Psi_0 = \prod_{|k| \le k_F} a_{k\uparrow}^{+} a_{k\downarrow}^{+} |0\rangle, \quad a_{k\sigma} = N^{-1/2} \sum_m c_{m\sigma} e^{ikma}, \tag{6}$$

where $k_F = \rho\pi/2a$. This state is unstable to a deformation of the type (2) with $Q = 2k_F$. The reason for the instability is that the expansion of the energy in powers of Δ contains a term proportional to $\Delta^2 \ln\Delta$, which minimizes the energy (5) at

$$\Delta \sim \exp(-1/b). \tag{7}$$

In the case $U \to \infty$ the system with Hamiltonian (1) can be regarded in the spinless-fermion approximation,[14-16] and then the wave function of the ground state is

$$\Psi = \prod_{|k| \le 2k_F} a_k^{+} |0\rangle. \tag{8}$$

Since all the levels with $|k| \le 2k_F$ are filled in the state (8), this state is unstable to a deformation of the type (2) with $Q = 4k_F$, but no instability to a deformation with $Q = 2k_F$ appears.[16]

The question is now whether the period of the deformation changes with changing U smoothly from λ_F to $\lambda_F/2$, or whether the two instabilities coexist at $U \neq 0$. An answer to this question is given in Ref. 19, in which it is shown that zero-gap excitation with $Q = 2k_F$ exists in a Hubbard chain at all values of U. The instability to deformations of type (2) can be attributed to singularities of the response function, and for such singularities to be present zero-gap excitations must exist. It follows therefore from the results of Ref. 19 that instability to

deformation with period λ_P takes place also at $U \neq 0$. What remains unanswered, however, is the question of the deformation with period $\lambda_P/2$ and the ratio of the responses to these deformations at finite values of the interaction parameter U.

We consider now the dependence of the ground-state energy (5) on the amplitude of the deformation (2) with $Q = 2k_F$ and $4k_F$, using for the calculation of the electron energy a procedure described in Ref. 17. The variational function used in Ref. 17 takes, when generalized to the case $\rho < 1$, the form

$$\Psi_g = \prod_{m=1}^{L} (f_{m\uparrow}^{+} f_{m\downarrow}^{+} \cos\alpha + \tilde{f}_{m\uparrow}^{+} \tilde{f}_{m\downarrow}^{+} \sin\alpha)\,|0\rangle, \tag{9}$$

where $\rho N = 2L \to \infty$ is the number of electrons, while the Fermi operators $f_{m\sigma}$ and $\tilde{f}_{m\sigma}$ correspond to the Wannier functions of the occupied and vacant subbands localized near the point $R_m = (m + \delta)\pi/k_F$:

$$f_{m\sigma} = \left(\frac{2}{N\rho}\right)^{1/2} \sum_{|k|<k_F} e^{-ikR_m} A_{k\sigma},$$
$$\tilde{f}_{m\sigma} = \left(\frac{2}{N\rho}\right)^{1/2} \sum_{|k|<k_F} e^{-ikR_m} \tilde{A}_{k\sigma}, \tag{10}$$

$$A_{k\sigma} = a_{k\sigma} \cos\theta_k + a_{\bar{k}\sigma} i \sin\theta_k,$$
$$\tilde{A}_{k\sigma} = a_{k\sigma} i \sin\theta_k + a_{\bar{k}\sigma} \cos\theta_k, \tag{11}$$

$\bar{k} = k - 2k_F \operatorname{sign} k$, while α and θ_k are variational parameters. The energy of the system per particle (in units of β) is

$$\varepsilon(\Delta) - U\rho/4 \equiv -\varepsilon_g(U, \Delta) = {}^1/_2 (t + \tilde{t}) + {}^1/_2 (t - \tilde{t}) \cos 2\alpha + {}^1/_2 I \sin 2\alpha, \tag{12}$$

where t and $\tilde{t}$ are the average values of the kinetic energy in the states f_m and $\tilde{f}_m$, respectively, and I is the matrix element of the interaction of the electrons between the states $f_{m\uparrow}^{+} f_{m\downarrow}^{+} |0\rangle$ and $\tilde{f}_{m\uparrow}^{+} \tilde{f}_{m\downarrow}^{+} |0\rangle$. Variation of the energy (12) with respect to the angle α leads to the relation[17]

$$\operatorname{tg} 2\alpha = I/(t - \tilde{t}). \tag{13}$$

As shown in Ref. 17, for the case $\rho = 1$ the function (9) describes correctly the dependence of the electron energy on U, does not violate the spin and charge symmetry of the system, and yields a lower ground-state energy than other variational calculations.

We examine now the dependence of the electron energy (12) on the parameter Δ [Eq. (4)] at different values of the parameter U. To simplify the analysis we assume that $\theta_k \equiv 0$ in (11). In this approximation $I = cU\rho/4$, where the constant c is of the order of unity. This choice of the parameter θ_k provides a good description of the energy of the ground state at $U < 1$. In the limit $U \to \infty$, the choice of f_m, and consequently of θ_k, becomes of great importance for the determination of the correct asymptotic form of the energy (12). In the next section we present one of the possible methods of choosing f_m for the cases $\rho = 1$ and $\rho = \frac{1}{2}$. As will be shown later, the choice of θ_k is not so important for our problem.

At $U = 0$, according to (10), (11), and (13), the function (9) goes over into the Slater determinant (6), and the energy (12) coincides with the average kinetic energy of the filled part of the band t. The dependence of t on the amplitude of the deformation (2) with $Q = 2k_F$ contains a term of the order of $\Delta^2 \ln\Delta$. It is also obvious that the dependence of the average kinetic energy $\tilde{t}$ ($k_F \leq |k| \leq 2k_F$) of the vacant subband on the amplitude of this deformation will be determined by a similar term, but with the sign reversed. A deformation of the type (2) with $Q = 4k_F$ leads to the appearance of a term logarithmic only in $\tilde{t}$ (the average kinetic energy of the vacant subband), since a gap appears in the single-particle spectrum under such a deformation at the points $k = \pm 2k_F$. Thus, if we neglect the dependence of the integral I on the amplitude of the deformation, then the electron energy (12) as a function of the deformation amplitude takes the form

$$\varepsilon(\Delta) - \varepsilon(0) = \eta(\Delta^2 \ln\Delta) \cos 2\alpha + O(\Delta^2) \quad (Q = 2k_F), \tag{14}$$

$$\varepsilon(\Delta) - \varepsilon(0) = \eta(\Delta^2 \ln\Delta) \sin^2\alpha + O(\Delta^2) \quad (Q = 4k_F), \tag{15}$$

where $\eta \approx 1$.

Using expressions (13) and (15) we arrive at the conclusion that an instability to deformation with $Q = 4k_F$ sets in even for a weak interaction ($U \ll 1$), but the leading term of the expansion of the electron energy in the deformation amplitude contains the small factor U^2. Therefore the equilibrium value of the amplitude of such a deformation, determined by the minimum of the expression (5), is

$$\Delta_0 \sim \exp(-1/bU^2). \tag{16}$$

In the same limit, as seen from (13) and (14), the response to a deformation with $Q = 2k_F$ depends little on U. In the other limit $U \gg 1$, the response to the deformation with $Q = 2k_F$ becomes weaker, inasmuch as according to (13) and (14) the principal term of the expansion of the electron energy in the amplitude of this deformation contains the factor U^{-1}, since $\cos 2\alpha \sim U^{-1}$.

We note here once more that estimates (14) and (15) given above are, generally speaking, valid only at small U. However, the conclusion drawn above concerning the presence of a factor U^{-1} in the leading term of the expansion (14) at $U \gg 1$ is confirmed both by the more complete analysis of this limit for the cases $\rho = 1$ and $\rho = \frac{1}{2}$, which will be given in the next section, and by the result of an investigation of an instability of the Peierls type in a Heisenberg chain of spins,[20-22] which is a good model for the description of a Mott-Hubbard one-dimensional system at $\rho = 1$ in the limit $U \to \infty$. In fact, the decrease of the energy of the ground state of the chain of spins is proportional to the exchange integral, which is equal to $4\beta^2/\gamma$ for a Hibbard chain.[11,12,14]

On the basis of expressions (14) and (15) one should expect the responses to deformations with $Q = 2k_F$ and $4k_F$ to be comparable in magnitude in the region of intermediate values of the parameters ($|I| \approx 2|t|$).

In the derivation of expressions (14) and (15) we have neglected the dependence of the integral I on the deformation amplitude. The existence of this dependence is due to the fact that when a deformation of type (2) is produced the band states near $k = \pm k_F$ become restructured. This restructuring leads to a strengthening of

the localization of the function (10), and consequently to an increase of the modulus of I. Allowance for these effects shows that they enhance the Peierls instability. This aspect of the problem is considered in greater detail in the next section for the case $\rho = 1$.

2. PARTICULAR CASES OF BAND FILLING: $\rho = 1$ AND $\rho = 1/2$

At $\rho = 1$, the system with Hamiltonian (1) is a Mott dielectric at any $U > 0$.[9-12,14] In this case the main values of the kinetic energy in (12) are connected by the relation $\tilde{t} = -t$.

Let us examine briefly the results for $U = 0$. The change of the resonant integrals of the type (3) causes a restructuring of the single-particle band states that enter in the function (6). It can be shown that this restructuring is determined by expression (11) provided that

$$2\theta_k = \operatorname{arctg}(z \operatorname{tg} k). \tag{17}$$

At $U = 0$, the energy is equal to the average kinetic energy t, which depends on z and on Δ:

$$\varepsilon(\Delta) = t(\Delta, z) = -4\pi^{-1}[E(1-z^2) + (\Delta - z)\partial E(1-z^2)/\partial z], \tag{18}$$

where $E(w)$ is a complete elliptic integral of the second kind. Variation of the expression (18) with respect to z yields $z = \Delta$ and the electron energy, as a function of Δ, takes the known form (see, e.g., Ref. 5)

$$t(\Delta, \Delta) = -\varepsilon_s(0,0) - \frac{2\Delta^2}{\pi}\left(\ln\frac{4}{\Delta} - {}^1/_2\right). \tag{19}$$

By varying the total energy (5) with respect to Δ, we obtain for the optimal value $\Delta = \Delta_0$

$$\Delta_0 = 4\exp(-\pi/4b). \tag{20}$$

If $U \neq 0$ and $\Delta = 0$, then it follows from the results of Ref. 17 that $\theta_k = 0$. A regular behavior of the energy (12) in the entire interval of values of U from zero to infinity can be obtained by choosing θ_k in (11) in the form (17). It follows therefore that the lattice deformation and the interaction of the electrons cause identical restructurings of the single-particle states. Therefore at $U \neq 0$ and $\Delta \neq 0$ the conversion parameter in (17) is $z > \Delta$. Let us explain this result qualitatively.

When the deformation amplitude increases, the parameter Δ increases and consequently also z in (9). The increase of z increases the localization of the Wannier functions (10) at the sites $2m$ and $2m+1$. In the limit as $z \to 1$ this localization becomes complete ($\theta_k \to k/2$).[17] Localization of the Wannier functions contained in the function (9) increases the exchange integral I in (12), i.e., decreases the energy of the system [$I = U/3$ at $\theta_k = 0$ and $I = U/2$ at $\theta_k = k/2$ (Ref. 17)].

Minimizing the energy (12) with respect to z for the case $U \ll 1$, we obtain

$$z - \Delta = -U^2/\ln\Delta > 0 \tag{21}$$

in accordance with the qualitative considerations advanced above. Neglecting the small correction to z in (21), we represent the dependence of the electron energy on Δ in the form

$$\varepsilon(\Delta) - U\rho/4 = -\varepsilon_s(0,\Delta) - I^2/8\varepsilon_s(0,0) - \frac{II'\Delta}{\varepsilon_s(0,0)}, \tag{22}$$

where I' is the derivative of the integral I with respect to z at $z = \Delta$. By virtue of the foregoing qualitative considerations, the product II' is positive. Therefore minimization of the total energy (5) with respect to Δ, with allowance for the dependence of the electronic component (23), yields a larger value of Δ at the minimum point than at $U = 0$ [see (20)]. Thus, the Peierls instability becomes stronger in the region of small values of the electron-interaction parameter.

In the case $U \gtrsim 4$, the value of the conversion parameter z depends little on Δ and is determined by the condition of the minimum of the electron energy (12). To obtain estimates in this region of values of U, we put $\theta_k = zk$. Then, taking (1), (3), and (9)–(12) into account, the average kinetic energy is

$$t(\Delta, z) = t(0, z)(1 + z\Delta). \tag{23}$$

The expansion of the electron energy takes the form

$$\varepsilon(\Delta) - \varepsilon(0) = zt^2(0, z)\Delta/\varepsilon_s(U, 0). \tag{24}$$

The value of the parameter z at $U \gtrsim 4$ is in the range $\frac{1}{4} \leqslant z \leqslant \frac{1}{2}$.[17] The minimum of the total energy (5), when (24) is taken into account, lies at

$$\Delta = zbt^2(0, z)/\varepsilon_s(U, 0). \tag{25}$$

It follows from (24) and (25) that the Peierls instability is preserved also in the region of large values of the interaction parameter. However, the response to the deformation becomes weaker because of the presence of the factor U^{-1} in the expansion of the energy in Δ (at $U \gg 1 \varepsilon_s \approx U/4$, Ref. 17).

We now consider the case of $\rho = \frac{1}{2}$, i.e., $k_F = \pi/4a$. To simplify the analysis, we assume that the functions (10) are fully localized on quartets of atoms (the index m in this case denotes the number of the quartet). This approximation is accurate enough, since the sum of the squares of the moduli of the quantities f_m over the atoms of the quartet amounts to approximately 0.8 even at $\theta_k = 0$ in (11). Optimization of the energy with respect to θ_k, as noted above, increases the localization. Therefore, in particular, the localized functions f_m describe the system better at larger values of the interelectron-interaction parameter. We represent the coefficients of the expansion of the functions f_m and $\tilde{f}_m$ over the atoms of the mth quartet in the form

$$f_m = \{v, u, u, v\}, \quad \tilde{f}_m = \{\tilde{v}, \tilde{u}, -\tilde{u}, -\tilde{v}\},$$

where $2(u^2 + v^2) = 1$. We express in terms of these coefficients the average kinetic-energy values that enter in (12):

$$t = -2uv(\beta_{12} + \beta_{34}) - u^2\beta_{23}, \tag{26}$$

$$\tilde{t} = -2\tilde{u}\tilde{v}(\beta_{12} + \beta_{34}) + \tilde{u}^2\beta_{23}. \tag{27}$$

The indices of the resonant integrals in (27) number the atoms of the quartet. A deformation of type (2) with $Q = 2k_F$ (quadrupling the period of the initial lattice) at $\varphi = \pi/4$ corresponds to a change of the resonant integrals of the form

$$\beta_{12}=\beta_{34}=\beta, \quad \beta_{23}=\beta(1+\Delta), \tag{28}$$

and when the period is doubled ($Q=4k_F$) we can put, in accordance with (3),

$$\beta_{12}=\beta_{34}=\beta(1+\Delta), \quad \beta_{23}=\beta(1-\Delta). \tag{29}$$

In the limit as $U\to\infty$, the need for excluding the contribution proportional to U in the energy (12) leads to the condition $u=v=\tilde{u}=\tilde{v}$. Using this condition and expressions (12), (26), and (27)–(29), we arrive at the conclusion that doubling of the period is energywise favorable. Quadrupling the lattice period decreases the electron energy by an amount proportional to β^2/γ, inasmuch as $\cos 2\alpha \approx U^{-1}$ according to (13). Consequently the response to a deformation with period λ_p decreases in this limit as a result of the presence of the factor U^{-1} in the leading term of the expansion of the electron energy in the deformation amplitude, in analogy with the case $\rho=1$ and in agreement with expression (15).

The case $\rho=1$ considered above was investigated previously also on the basis of another variational approach, which is customarily called the method of different orbitals for different spins, or the generalized Hartree-Fock method (GHFM).[14] It was just in this approximation that the dielectric character of the spectrum of the system was first deduced.[9] The question of the instability to doubling of the period within the framework of the GHFM can be investigated only numerically. The corresponding calculations (see the review[14] and Refs. 23–25) show that the interelectron interaction suppresses partially ($U\ll 1$) or completely ($U>1$) the Peierls instability. The conclusions obtained in the present paper agree qualitatively with the results of the GHFM only in the limit $U\gg 1$. In this limit, according to (24) or (14), the leading term of the expansion of the energy contains the small factor U^{-1}, i.e., the instability becomes weaker, although it is not completely suppressed. On the other hand, according to our results, the Peierls instability does not become weaker in the case of a weak interaction.

We present a number of arguments that enable us to estimate the degree of accuracy of the results obtained by us on the basis of the approximation (9). In the limit $U\ll 1$, the leading term of the expansion of the energy (12) in powers of U in the absence of deformation ($\Delta=0$) differs from the exact solution only by a factor ≈ 1.[17] On this basis one can assume that at $U\ll 1$ the results obtained with the aid of the function (9) are reliable. In the case of strong interaction ($U\gg 1$) both the function (9) and the GHFM function give practically the same asymptotic expression for the energy.[17] As noted above, comparison with the results of an investigation of Peierls instability in a spin chain[21,22] leads to the conclusion that the weakening of the instability in the strong-interaction limit is connected with the presence of the factor U^{-1} in the expansion of the energy in the deformation amplitude, as is the case in expressions (14) and (24). Favoring the presence of an instability of the Peierls type at $U>1$ is also the presence, established by exact calculations, of zero-gap excitations with $Q=2k_F$ in the spectrum of the system for all values of U.[11,12,19] This point of view agrees also with the experimentally observed doubling of the period of the TCNQ chains in TCNQ complexes with alkali metals.[8] Such a system is a Mott dielectric with a large (≈ 1 eV) gap in the spectrum of the current excitation.[26]

The foregoing data show that the approach used in the present paper accounts well, on the whole, for the dependence of the energy of the ground state (5) on the amplitude of the Peierls deformation: at $U\ll 1$ the value of Δ which minimizes (5) depends weakly on U, and the Peierls instability decreases smoothly with increasing U, but vanishes only in the limit $U\to\infty$ (and not at finite values of U as when the GHFM is used[23]). At the same time, the change from a dependence of the type $\Delta^2\ln\Delta$ to a linear function of Δ in the expansion of the electron energy (12) can be attributed to the approximate calculation method used by us. In other words, in the case of the exact solution the form of the expansion (14) may either be preserved or may contain a linear term as well as a logarithmic one.

From the methodological point of view it is of interest to note also the following. The permutation symmetry of the spatial part of the function (9) corresponds to a Young pattern with line-cell numbers making up the natural series. The spatial symmetry of the GHFM function is characterized by a Young pattern with maximum possible deviation of the cell numbering from the natural sequence.[27] Thus, the GHFM function and the function (9) correspond to two extreme cases of permutation symmetry. One must therefore expect the exact solution to have intermediate properties. As follows from the foregoing, this is precisely the situation realized with respect to the Peierls instability: within the GHFM framework the contribution of the Peierls deformation to the energy is underestimated, whereas the use of the function (9) seems to overestimate somewhat this contribution, ($U\gg 1$).

CONCLUSION

We call attention to a number of consequences of the analysis performed in the present paper. According to expressions (14) and (24), the value of the amplitude of the Peierls deformation, which minimizes the total energy of the ground state, remains finite at all finite values of U. It follows therefore that a one-dimensional Mott dielectric is unstable to lattice deformation at all values of the interaction parameter. In other words, Mott and Peierls instabilities coexist. This conclusion explains the presence of static Peierls deformation at low temperatures in TCNQ complexes with alkali metals[8]—Mott dielectrics with large gap in the current-excitation spectrum.[26] Let us estimate, on the basis of x-ray structure data, the electron-phonon interaction constant b, which enters in (5), for one such crystal, namely Rb-TCNQ. According to low-temperature measurements,[28] the alternating interstitial distances in the TCNQ chain are 3.77 and 3.42 Å. Therefore, the amplitude of the deformation is $ax=0.18$ Å and $x=0.5$. Putting $\beta' a/\beta=1$ in (3), we get $\Delta=0.05$. Taking (25) into account, we next obtain $b=0.3-0.15$ (at $U\gtrsim 4$ we have $\frac{1}{4}\leqslant z\leqslant\frac{1}{2}$, Ref. 17). Expression (20), which is valid at $U=0$, yields, $b\approx 0.2$. In this case both expressions lead

to quantities of the same order (we have assumed that $U \approx 4$). If $\beta' a/\beta = 0.1$, then we find on the basis of (25) that $b = 0.015$–0.013, and from (20) it follows that $b \approx 0.1$. An estimate of b from the relation $b = (\beta')^2/\beta M\omega^2$ using the TCNQ mass and Debye temperature $\Theta_D = 100$ K leads to a value $b \approx 10^{-2}$.

The foregoing analysis of expression (14) and (15) leads also to the conclusion that at medium values of the electron-interaction parameter U a one-dimensional system with Hamiltonian (1) is unstable to periodic deformations of the type (2) with $Q = 2k_F$ and $Q = 4k_F$. In experiments on x-ray scattering by the quasi-one-dimensional crystal TTF-TCNQ,[18] characteristic symptoms of instability to both deformations were observed, and the x-ray scattering amplitudes were comparable in magnitude for $Q = 2k_F$ and $Q = 4k_F$. In light of our analysis this means that the effective interelectron interaction in this crystal is of the order of (or larger than) the width of the conduction band (0.5 eV, Ref. 29).

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Multiphoton boundary of the excitation spectrum in He II

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The behavior of the dynamic form factor in He II near the sound line $\omega = up$ is obtained. General formulas are derived for the asymptotic forms of the imaginary parts of the Green's function at high frequencies and large momenta.

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1. FORMULATION OF PROBLEM. KINEMATIC RELATIONS

The purpose of the present study was to investigate the decay of elementary excitations into phonons in superfluid helium in the case when the conservation laws permit such a decay only simultaneously into a large number of phonons.

It is known (see, e.g., Ref. 1) that at small momen-

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