

Peierls-Fröhlich problem in the continuum approximation

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The exact solution of the Peierls-Fröhlich problem on a self-consistent state of conduction electrons and a chain deformation near zero temperature is obtained in the continuum approximation. The charge-density-wave (CDW) state in various relations between parameters of the problem (electron density, electron-phonon coupling, CDW velocity) is investigated. The CDW total energy and momentum are calculated and an expression for the effective mass is obtained. Current oscillations are interpreted on the basis of this exact solution.

I. INTRODUCTION

A self-consistent state of the conduction electrons and lattice deformation in a one-dimensional metal was considered by Fröhlich in 1954.¹ This state was then called the charge density wave (CDW) and today it is widely studied both theoretically and experimentally.²⁻⁹ The Fröhlich assumption that only one phonon mode with the wave number $q=2k_F$ (k_F is the Fermi wave number) is occupied macroscopically and interacts strongly with electrons is often used for the explanation of certain properties of the CDW. But it has been proved during the last decade that continuum Peierls-Fröhlich models have exact solutions. The model with linearized dispersion law of electrons near Fermi level⁶⁻⁸ that describes systems with nearly half-filled bands such as doped *trans*-polyacetylene, and Fröhlich model with quadratic dispersion law^{4,5} which is applicable in the case of relatively small density of the carriers when the effective-mass approximation may be used, have been investigated. Moreover, exactly soluble discrete Peierls models have been found.⁹

In previous papers the static CDW was the main object of investigation. But the CDW can propagate as the whole entity along the chain with some velocity V , that corresponds to a certain value of its total momentum and the existence of current, $j_{CDW}=eN_e V$ (e being the electron charge and N_e being a number of electrons), in the chain. The possibility of such a type of CDW conductivity was indicated by Fröhlich¹ and there are up-to-date experimental investigations of the "sliding-mode" conductivity in CDW materials, as NbSe₃, TaS₃, etc. (see, for example, Grüner's review³). The sliding-mode conductivity is often characterized by some peculiarities; therefore the study of the exactly soluble Peierls-Fröhlich problem with account of CDW motion along the chain continues to command interest.

The present paper deals with the continuum Fröhlich model with a quadratic dispersion law. The exact spectrum of single-electron states in CDW and corresponding wave functions are found. CDW total energy and momentum are calculated. The Fröhlich approximation is shown to be valid only for small velocities of CDW

motion and for relatively high electron density. For small electron density or large velocity of the motion, CDW represents a set of periodically distributed bisolitons considered by Davydov and Brizhik.¹⁰ The analysis of the exact solution evidently shows the presence of $\nu_n=\nu n$ harmonics with decreased amplitudes, in addition to the fundamental frequency ν , in current oscillations spectrum, often called narrow-band noise (NBN).³

II. SELF-CONSISTENT EQUATIONS

Let us consider a chain with an atom in the unit cell and assume that the principal region of the chain of length $L=Na$ (a is the lattice constant) has N_e conduction electrons. In the continuum approximation without account of the Coulomb interaction between electrons, a system of N_e electrons interacting with the lattice vibrations is described by the Fröhlich Hamiltonian¹

$$\mathcal{H} = \sum_{j=1}^{N_e} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \frac{1}{\sqrt{N}} \sum_q g(q) e^{iqx_j} (b_q + b_{-q}^\dagger) \right] + \sum_q \hbar V_s |q| b_q^\dagger b_q. \quad (2.1)$$

Here m is the effective electron mass in the conduction band, b_q (b_q^\dagger) are the phonon creation (annihilation) Bose operators with the wave number q , $V_s = a(w/M)^{1/2}$ is the sound velocity in the chain, M is atom mass, w is the elasticity coefficient, and

$$g(q) = 2iga \left[\frac{\hbar}{2MV_s} \right]^{1/2} \frac{q}{\sqrt{|q|}}, \quad (2.2)$$

where g is the parameter of deformation short-range interaction of the electron with atom displacements.

To find out the wave function Ψ of the system we make use of the variational method. It is then taken into account that the total momentum operator

$$\mathcal{P} = - \sum_{j=1}^{N_e} i\hbar \frac{\partial}{\partial x_j} + \sum_q \hbar q b_q^\dagger b_q \quad (2.3)$$

commutes with the Hamiltonian (2.1). If we take interest in the state of the system with a certain value of the total

momentum, the wave function should be found from the condition of functional extremum¹

$$\mathcal{F} = \langle \Psi | (\mathcal{H} - VP - \varepsilon N_e) | \Psi \rangle, \quad (2.4)$$

where ε and V are Lagrange multipliers.¹¹

The wave function of the system Ψ , dependent on the electron and vibrational variables, is written as

$$\Psi(\{\tau_j\}, \{b_q^\dagger\}) = \exp \left[i \frac{mV}{\hbar} \sum_{j=1}^{N_e} x_j \right] \Phi(\{\tau_j\}) e^S |0\rangle, \quad (2.5)$$

where

$$S = \sum_q (\beta_q b_q^\dagger - \beta_q^* b_q). \quad (2.6)$$

Here $|0\rangle$ is the phonon vacuum state, β_q are variational parameters, and $\tau_j \equiv \{x_j, \sigma_j\}$ is the electron coordinate involving both the space x_j and spin σ_j variables.

Using Eq. (2.5) we find the functional (2.4)

$$\mathcal{F} = \int \Phi^* \left\{ \sum_{j=1}^{N_e} H(x_j) + \sum_q \hbar(V_s |q| - Vq) \beta_q^* \beta_q - (\varepsilon + \frac{1}{2} mV^2) \right\} \Phi d\tau, \quad (2.7)$$

where

$$H(x_j) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + U(x_j) \quad (2.8)$$

is one-electron Schrödinger operator with the potential

$$U(x) = \frac{1}{\sqrt{N}} \sum_q g(q) (\beta_q + \beta_{-q}^*) e^{iqx} \quad (2.9)$$

generated by lattice deformation;

$$d\tau = \prod_{j=1}^{N_e} d\tau_j, \quad \int (\dots) d\tau_j = \sum_{\sigma_j = \pm 1} \int_{-L/2}^{L/2} (\dots) dx_j.$$

Taking into account the additivity one-electron operators in Eq. (2.7) one can represent a multielectron function Φ as a determinant

$$\Phi(\{\tau_j\}) = \frac{1}{\sqrt{N_e!}} \det \left| \varphi_i(\tau_j) \right|, \quad i, j = 1, 2, \dots, N_e, \quad (2.10)$$

where

$$\varphi_l(\tau) = \Psi_\lambda(x) \chi_\mu(\sigma), \quad l \equiv \{\lambda, \mu\} \quad (2.11)$$

are the orthonormalized one-electron wave functions

$$\begin{aligned} \int \varphi_l^*(\tau) \varphi_{l'}(\tau) d\tau &= \sum_{\sigma = \pm 1} \chi_\mu^*(\sigma) \chi_\mu(\sigma) \\ &\quad \times \int_{-L/2}^{L/2} \Psi_\lambda^*(x) \Psi_{\lambda'}(x) dx \\ &= \delta_{ll'} = \delta_{\mu\mu'} \delta_{\lambda\lambda'}. \end{aligned}$$

$\chi_\mu(\sigma)$ is the spin wave function of the electron ($\mu = \pm 1$).

Using the independent variations of the functional (2.7) by the parameters β_q and the electron wave functions we get a system of equations

$$\beta_q = -\frac{1}{\sqrt{N}} \frac{g^*(q) f(q)}{\hbar(V_s |q| - Vq)}, \quad (2.12)$$

$$H\Psi_\lambda \equiv \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \Psi_\lambda = \mathcal{E}_\lambda \Psi_\lambda, \quad (2.13)$$

where

$$f(q) = \sum_{j=1}^{N_e} \int \Phi^* e^{-iqx_j} \Phi dt = \int_{-L/2}^{L/2} e^{-iqx} \rho_1(x) dx, \quad (2.14)$$

$$\rho_1(x) = \sum_\lambda n_\lambda |\Psi_\lambda(x)|^2. \quad (2.15)$$

Here n_λ is the number indicating how many times (generally 1 or 2) the coordinate function Ψ_λ is included in the determinant (2.10).

If we substitute (2.12) into (2.9) with allowance for (2.14) we get the following expression for the self-consistent potential:

$$U(x) = -\frac{4g^2 a}{w(1-s^2)} \rho_1(x) = -\frac{4g^2 a}{w(1-s^2)} \sum_\lambda n_\lambda |\Psi_\lambda(x)|^2, \quad (2.16)$$

where $s = V/V_s$ is the ratio between the velocity V and the sound velocity V_s . Thus having excluded the vibrational variables we get the system of nonlinear differential equations

$$\frac{\hbar^2}{2m} \frac{d^2 \Psi_\lambda}{dx^2} + \frac{4g^2 a}{w(1-s^2)} \sum_{\lambda'} n_{\lambda'} |\Psi_{\lambda'}|^2 \Psi_\lambda + \mathcal{E}_\lambda \Psi_\lambda = 0 \quad (2.17)$$

for the coordinate one-electron wave functions incoming in the determinant (2.10).

In the case of one electron ($n_s = 1$) we have a nonlinear equation describing the soliton state of the electron in the deformable chain.¹² One equation will also be obtained if we consider the lowest in energy singlet state of two electrons with opposite spins ($n_{bs} = 2$) which corresponds to the bisoliton state considered by Davydov and Brizhik.¹⁰ In the general case of N_e electrons in the ground state when states \mathcal{E}_λ lowest in energy are occupied by two electrons with the opposite spins ($n_\lambda = 2$), (2.17) is a system of $N_e/2$ equations (N_e is assumed to be even).

The total momentum and total energy of the system of electrons in the state (2.5) will be equal to

$$P = \langle \Psi | \mathcal{P} | \Psi \rangle = mVN_e + \sum_q \hbar q |\beta_q|^2 + \sum_\lambda n_\lambda \bar{p}_\lambda, \quad (2.18)$$

$$E = \langle \Psi | \mathcal{H} | \Psi \rangle$$

$$= \frac{1}{2} mV^2 N_e + \sum_\lambda n_\lambda \mathcal{E}_\lambda + \sum_q \hbar V_s |q| |\beta_q|^2 + V \sum_\lambda n_\lambda \bar{p}_\lambda \quad (2.19)$$

where

$$\bar{p}_\lambda = -i\hbar \int_{-L/2}^{L/2} \Psi_\lambda^* \frac{d\Psi_\lambda}{dx} dx \quad (2.20)$$

is the quantum-mechanical average of the electron momentum in the state Ψ_λ .

III. SELF-CONSISTENT POTENTIAL

A system of differential equations (2.17) allows for the exact solution.⁵ To find it and to determine in a self-consistent manner its constants we shall notice that the system of equations (2.17) has the first integral of the form

$$\frac{\hbar^2}{2m} \sum_\lambda n_\lambda \left| \frac{d\Psi_\lambda}{dx} \right|^2 + \sum_\lambda n_\lambda \mathcal{E}_\lambda |\Psi_\lambda|^2 + \frac{2g^2a}{w(1-s^2)} \left(\sum_\lambda n_\lambda |\Psi_\lambda|^2 \right)^2 = C_1, \quad (3.1)$$

where C_1 is the integration constant.

Differentiating the equality (2.16) twice taking account the equations (2.17) and the first integral (3.1) we find

$$\frac{d^2U}{dx^2} = \frac{6m}{\hbar^2} U^2 + \frac{32mg^2a}{\hbar^2 w(1-s^2)} \sum_\lambda n_\lambda \mathcal{E}_\lambda |\Psi_\lambda|^2 - \frac{16mg^2a}{\hbar^2 w(1-s^2)} C_1. \quad (3.2)$$

Taking into consideration (2.16) we assume the following relation to be fulfilled:

$$\frac{8mg^2a}{\hbar^2 w(1-s^2)} \sum_\lambda n_\lambda \mathcal{E}_\lambda |\Psi_\lambda|^2 = BU(x) + \frac{\hbar^2}{2m} A, \quad (3.3)$$

where unknown constants A and B should be determined in a self-consistent way on finding out the solution.

Thus, the assumption (3.3) leads to the nonlinear equation for the potential

$$\frac{d^2U}{dx^2} = \frac{6m}{\hbar^2} U^2 + 4BU - \frac{\hbar^2}{m} C. \quad (3.4)$$

Here the notation is introduced

$$C = \frac{16m^2g^2a}{\hbar^4 w(1-s^2)} C_1 - 2A. \quad (3.5)$$

The first integration of Eq. (3.4) gives

$$\left[\frac{dU}{dx} \right]^2 = \frac{4m}{\hbar^2} U^3 + 4BU^2 - \frac{2\hbar^2}{m} CU + \frac{2\hbar^2}{m^2} \mathcal{D} \quad (3.6)$$

with \mathcal{D} being the integration constant. By means of substitution

$$U(x) = \frac{\hbar^2}{m} [F(x) - \frac{1}{3}B] \quad (3.7)$$

the third power polynomial relative to U in the right-hand side Eq. (3.6) is reduced to a normal Weierstrass form, and for the function $F(x)$ we get from (3.6) the equation

$$\left[\frac{dF}{dx} \right]^2 = 4F^3 - g_2F - g_3 = 4(F - e_1)(F - e_2)(F - e_3). \quad (3.8)$$

Here e_i ($i = 1, 2, 3$) are roots for the cubic equation

$$4t^3 - g_2t - g_3 = 0 \quad (3.9)$$

with invariants

$$g_2 = \frac{4}{3}B^2 + 2C \quad (3.10a)$$

$$g_3 = -\left(\frac{8}{27}B^3 + \frac{2}{3}BC + 2\mathcal{D}\right). \quad (3.10b)$$

Hence, the problem of finding the self-consistent potential is reduced to the integral inversion problem

$$x = \int_{F(0)}^F \frac{dt}{(4t^3 - g_2t - g_3)^{1/2}}$$

which is solved in the Weierstrass elliptic function $\wp(z)$.¹³ Here and further we shall use the standard notation for the theory of elliptic functions.^{13,14}

The self-consistent potential by definition (2.16) is the real and bounded function of the coordinate x . Thus, Eq. (3.8) will be physically meaningful only when the discriminant $g_2^3 - 27g_3^2$ of the cubic equation (3.9) is positive and all three roots e_i are real and different. The solution to Eq. (3.6) will then be written as

$$U(x) = \frac{\hbar^2}{m} [\wp(x + \omega') - \frac{1}{3}B]. \quad (3.11)$$

The elliptic Weierstrass function $\wp(z)$ is doubly periodic function with periods denoted as 2ω and $2\omega'$. In the elliptic function theory^{13,14} the symmetric notations are generally used

$$\omega_1 = \omega, \quad \omega_2 = -\omega - \omega', \quad \omega_3 = \omega'.$$

Then $\wp(\omega_i) = e_i$ ($i = 1, 2, 3$). With positive discriminant, $g_2^3 - 27g_3^2 > 0$, the real roots for the cubic equation (3.9) are distributed as follows:

$$e_1 > e_2 > e_3$$

and

$$e_1 > 0, \quad e_3 < 0.$$

In this case the period $2\omega_1 = 2\omega$ is real, and $2\omega_3 = 2\omega'$ is purely imaginary.

Thus, a one-dimensional system of electrons, deforming the lattice, generates for itself a periodic potential (3.11) with the period $2\omega_1$.

IV. EIGENFUNCTION AND ELECTRON SPECTRUM IN SELF-CONSISTENT POTENTIAL

To make the problem self-consistent by using the relations (2.16) and (3.3) it is necessary to find the eigenfunctions and the eigenvalues of Schrödinger equation (2.13). Taking into account the explicit form (3.11) of the self-consistent potential we rewrite the equation (2.13) as

$$\frac{d^2\Psi}{dx^2} + \left[\frac{2m}{\hbar^2} \mathcal{E} + \frac{2}{3}B - 2\wp(x + \omega_3) \right] \Psi = 0. \quad (4.1)$$

This equation is a particular case of the Lamé equation,^{13,14} written in the Weierstrass form

$$\frac{d^2\Psi}{dz^2} = [n(n+1)\wp(z) - \Lambda]\Psi \quad (4.2)$$

when

$$n = 1, \quad \Lambda = \frac{2m}{\hbar^2} \mathcal{E} + \frac{2}{3}B, \quad z = x + \omega_3. \quad (4.3)$$

The Lamé potentials refer to a class of finite-band potentials,^{15,16} i.e., they have in their spectrum a finite number [equal to the number n in (4.2)] of the forbidden bands (gaps). Consequently, a self-consistent potential (3.11) is a single-gap potential.

The fact that the electrons deforming the chain create the single-gap potential for themselves is one of the main results of the Peierls-Fröhlich problem exact solution.⁴⁻⁸ The electron band structure and eigenfunctions in this case are well known.^{5,8,15-17} In Refs. 5, 8, and 17 the Lamé equation was written in Jacobi form, instead we shall use Weierstrass form and write its solution via Weierstrass σ function¹³ in the form satisfying the Bloch theorem

$$\Psi_k(x) = e^{ikx} U_k(x) = e^{-[\zeta(\lambda) - (\eta_1/\omega_1)\lambda]x} U_\lambda(x), \quad (4.4)$$

$$U_\lambda(x) = A_\lambda \frac{\sigma(x + \omega_3 + \lambda)}{\sigma(x + \omega_3)} e^{-(\eta_1/\omega_1)\lambda x}, \quad (4.5)$$

where A_λ is the normalized constant, $\sigma(z)$ and $\zeta(z)$ are Weierstrass σ and ζ functions, η_1 is the standard constant of the elliptic function theory: $\eta_i = \zeta(\omega_i)$; $i = 1, 2, 3$, and λ is an arbitrary constant—the parameter of the solution.

By virtue of Weierstrass σ -function properties the function (4.5) is a periodic function with the period $2\omega_1$ equal to the period of the potential (3.11). Thus, the wave function (4.4) is an eigenfunction of the translation operator at the distance multiple to the period of the potential, with corresponding eigenvalue $\exp\{-[\zeta(\lambda) - \eta_1\lambda/\omega_1]2\omega_1 n\}$. Hence the combination

$$k = i \left[\zeta(\lambda) - \frac{\eta_1}{\omega_1} \lambda \right] \quad (4.6)$$

has the sense of the wave number.

The eigenvalues of Eq. (4.1) are determined by the parameter λ and equal to

$$\mathcal{E}_\lambda = -\frac{\hbar^2}{2m} \left[\frac{2}{3}B + \wp(\lambda) \right]. \quad (4.7)$$

The relations (4.6) and (4.7) give in the parametric form (via the parameter λ) the electron state spectrum in the periodic potential (3.1). As is known, in the one-dimensional case extremums of the function $\mathcal{E}(k)$ correspond to the center ($k=0$) and to the edge ($k=\pm\pi/2\omega_1$) of the Brillouin zone of periodic potential. We find from (4.7) and (4.6)

$$\frac{d\mathcal{E}}{dk} = \frac{d\mathcal{E}/d\lambda}{dk/d\lambda} = \left[\frac{2\hbar^2}{m} \right]^{1/2} \frac{\sqrt{Q(\mathcal{E})}}{\left| \mathcal{E} - \frac{\hbar^2}{2m} \left[\frac{\eta_1}{\omega_1} - \frac{2}{3}B \right] \right|}, \quad (4.8a)$$

$$Q(\mathcal{E}) = \left[\mathcal{E} + \frac{\hbar^2}{2m} (e_1 + \frac{2}{3}B) \right] \left[\mathcal{E} + \frac{\hbar^2}{2m} (e_2 + \frac{2}{3}B) \right] \times \left[\mathcal{E} + \frac{\hbar^2}{2m} (e_3 + \frac{2}{3}B) \right]. \quad (4.8b)$$

Hence, the polynomial zeros (4.8b) determine the energy-band boundaries in the electron spectrum

$$\mathcal{E}_1 = -\frac{\hbar^2}{2m} (e_1 + \frac{2}{3}B), \quad \mathcal{E}_2 = -\frac{\hbar^2}{2m} (e_2 + \frac{2}{3}B), \quad (4.9)$$

$$\mathcal{E}_3 = -\frac{\hbar^2}{2m} (e_3 + \frac{2}{3}B)$$

where $e_1 > e_2 > e_3$ and $e_1 > 0$, $e_3 < 0$.

Thus, in the spectrum of Schrödinger equation (4.1) there are two regions of allowed energies [$Q(\mathcal{E}) \geq 0$]: $\mathcal{E}_1 \leq \mathcal{E} \leq \mathcal{E}_2$ and $\mathcal{E} \geq \mathcal{E}_3$ which are separated by a forbidden band [$Q(\mathcal{E}) < 0$] $\mathcal{E}_2 < \mathcal{E} < \mathcal{E}_3$. To write the Bloch wave functions (4.5) and the corresponding dispersion laws for each of the allowed bands it is necessary to determine the parameter λ values admissible physically. The condition of \mathcal{E} and k being real in virtue of the Weierstrass functions properties leads to the parameter λ being equal to

$$\lambda = \lambda_\nu(\alpha) = i\alpha + \nu\omega_1, \quad (4.10)$$

where α can take arbitrary values on the real axis, and ν is integer. Two energy branches (4.7) as the functions of the parameter α respond to these values of the parameter λ . The odd values $\nu=1, 3, \dots$ correspond to the lower allowed band with the energy $\mathcal{E}_1 \leq \mathcal{E}_1(\alpha) \leq \mathcal{E}_2$ and the even $\nu=0, 2, \dots$ —to the upper one with the energy $\mathcal{E}_0(\alpha) \geq \mathcal{E}_3$.

Thus, in Eqs. (4.4)–(4.7), according to (4.10), the parameter λ is the double quantum number $\lambda \equiv \{\nu, \alpha\} = \{\nu, k\}$ that determines the number of the allowed band, ν , and the state inside the band—either α or k , in view of their single-valued correspondence. Since Eqs. (4.4)–(4.7) are independent of n both for even $\nu=2n$ and odd $\nu=1+2n$ values ν , we restrict the number ν in (4.10) to taking only two values 0 and 1. The value $\nu=0$ corresponds to the upper allowed band with the dispersion law (4.6) and (4.7) when $\lambda = \lambda_0(\alpha) = i\alpha$ and $\nu=1$ to the lower one with the dispersion law (4.6)–(4.7) for $\lambda = \lambda_1(\alpha) = i\alpha + \omega_1$. With allowance for periodicity of the Weierstrass function $\wp(z)$ in the imaginary axis with period $2\omega_3 = 2\omega'$ the value of α will be bounded by the main region

$$-\omega_3 < i\alpha \leq \omega_3 \quad \text{or} \quad -\bar{\omega}_1 < \alpha \leq \bar{\omega}_1, \quad (4.11)$$

where $\omega_1 = -i\omega_3$. In the space of the wave vectors this choice corresponds to a scheme of the broadened band.^{8,17} For the lower allowed band, $\nu=1$, with varying α in the region (4.11), the wave number (4.6) takes the value in the first Brillouin zone:

$$-\pi/2\omega_1 < k \leq \pi/2\omega_1.$$

Then

$$\mathcal{E}_1(\alpha=0) = \mathcal{E}_1(k=0) = \mathcal{E}_1$$

and

$$\mathcal{E}_1(\alpha = \pm \tilde{\omega}_1) = \mathcal{E}_1(k = \pm \pi/2\omega_1) = \mathcal{E}_2.$$

For the upper band, $\nu=0$, the region of wave number one values (4.6) will be $|k| \geq \pi/2\omega_1$ and the energy takes the value

$$\mathcal{E}_0(\alpha = \pm \tilde{\omega}_1) = \mathcal{E}_0(k = \pm \pi/2\omega_1) = \mathcal{E}_3$$

and

$$\mathcal{E}_0(k) = -\frac{\hbar^2 B}{3m} + \frac{\hbar^2 k^2}{2m}$$

at

$$|k| \gg \pi/2\omega_1$$

when $|\alpha| \ll \tilde{\omega}_1$.

The normalized constants, $A_\nu(k) \equiv A_\nu(\alpha)$, determines from the normalization conditions for the wave functions (4.4), will be equal to

$$A_1(\alpha) = \frac{1}{\sqrt{L}} \left[\frac{\rho(i\alpha + \omega_1) - e_2}{\rho(i\alpha + \omega_1) + \frac{\eta_1}{\omega_1}} \right]^{1/2} \times \frac{e^{-\eta_1 \omega_1} \sigma(\omega_3)}{\sigma(\omega_1) \sigma(i\alpha + \omega_3)} (e_1 - e_2)^{-1/2}, \quad (4.12)$$

$$A_0(\alpha) = \frac{1}{\sqrt{L}} \left[\frac{\rho(i\alpha) - e_3}{\rho(i\alpha) + \frac{\eta_1}{\omega_1}} \right]^{1/2} \frac{\sigma(\omega_3)}{\sigma(i\alpha + \omega_3)}. \quad (4.13)$$

V. SELF-CONSISTENCY

To determine the unknown constants it is necessary to make the equations obtained self-consistent. Knowing this while using the explicit form of the solutions we have to require the equalities (2.16) and (3.3) to be satisfied identically. This leads to the following three self-consistency conditions:

$$\frac{1}{L} \sum_{\nu, k} \frac{n_{\nu, k}}{D_\nu(k)} = -\frac{1}{\kappa}, \quad (5.1)$$

$$\frac{1}{L} \sum_{\nu, k} n_{\nu, k} \frac{B + \frac{2m}{\hbar^2} \mathcal{E}_\nu(k)}{D_\nu(k)} = 0, \quad (5.2)$$

$$\frac{1}{L} \sum_{\nu, k} n_{\nu, k} \frac{2m}{\hbar^2} \mathcal{E}_\nu(k) \frac{\left[B + \frac{2m}{\hbar^2} \mathcal{E}_\nu(k) \right]}{D_\nu(k)} = \frac{1}{2\kappa} A, \quad (5.3)$$

where the notations are introduced

$$D_\nu(k) \equiv D_\nu(\alpha)$$

$$= \frac{2}{3} B - \frac{\eta_1}{\omega_1} + \frac{2m}{\hbar^2} \mathcal{E}_\nu(k) = - \left[\frac{\eta_1}{\omega_1} + \rho(\lambda_\nu) \right], \quad (5.4)$$

$$\kappa = \frac{\kappa_0}{1-s^2}, \quad \kappa_0 = \frac{4mg^2 a}{\hbar^2 w}. \quad (5.5)$$

Of the whole complete set of orthonormalized functions (4.4) only the functions involved in the determinant (2.10) come into the relations (2.16) and (3.3). Thus, in calculating the sums in Eqs. (5.1)–(5.3) we assume the numbers $n_{\nu, k}$ to be the occupation numbers. For the ground state at zero temperature $n_{\nu, k} = n[\mathcal{E}_\nu(k)] = 2$ for the occupied states and $n[\mathcal{E}_\nu(k)] = 0$ for the empty ones. Then the conditions (5.1)–(5.3) should be supplemented by the fourth condition

$$\sum_{\nu, k} n_{\nu, k} = N_e. \quad (5.6)$$

With account of the explicit form $D_\nu(k)$ and the equalities (5.1) and (5.6), the condition (5.2) can be reduced to

$$\frac{\eta_1}{\omega_1} + \frac{1}{3} B = \frac{2k_F \kappa}{\pi}, \quad (5.7)$$

where $k_F = \pi n_e / 2a$ is the Fermi wave number of free electrons; $n_e = N_e / N$ is the electron concentration in the chain. In calculating sums it is useful to go to integrating over the parameter α ;¹⁸ the condition (5.6) then takes the form

$$k(\bar{\lambda}_\nu) \equiv i \left[\xi(\bar{\lambda}_\nu) - \frac{\eta_1}{\omega_1} \bar{\lambda}_\nu \right] = k_F. \quad (5.8)$$

Here $\bar{\lambda}_\nu = \lambda_\nu(\alpha_0)$ where α_0 is the value of parameter α that determines the boundary energy of the electrons $\mathcal{E}_\nu(\alpha_0) = \mathcal{E}_F$. Then $\nu=1$ in the case of complete or partial filling of the low band up to the energy $\mathcal{E}_1(\alpha_0)$ and $\nu=0$ when the low band is occupied completely and the upper one—up to the energy $\mathcal{E}_0(\alpha_0)$. The value of the parameter α_0 follows directly from the condition (5.1)

$$\alpha_0 = \frac{\pi}{2\kappa}. \quad (5.9)$$

With allowance for the Legendre relations^{13,14} the analysis of equalities (5.7) and (5.8) shows that they transform into the identity at

$$\frac{1}{3} B = -\frac{\eta_3}{\omega_3} \equiv -\frac{\eta'}{\omega'}, \quad (5.10)$$

$$\omega_1 \equiv \omega = \frac{\pi}{2k_F}, \quad (5.11)$$

$$\omega_3 \equiv \omega' = \frac{i\pi}{2\kappa} = i\alpha_0. \quad (5.12)$$

For the constant A introduced in (3.3) and the constants C_1 and \mathcal{D} we find the following values from the condition (5.3) and the definitions (3.10a) and (3.10b):

$$A = -\frac{4m\kappa}{\hbar^2} C_1, \quad C_1 = \frac{\hbar^2}{2m\kappa} \left[\frac{1}{12} g_2(\omega, \omega') - \left[\frac{\eta'}{\omega'} \right]^2 \right], \quad (5.13a)$$

$$\mathcal{D} = -\frac{1}{2} \left[g_3(\omega, \omega') - \frac{\eta'}{\omega'} g_2(\omega, \omega') + 4 \left[\frac{\eta'}{\omega'} \right]^3 \right]. \quad (5.13b)$$

Thus, in a one-dimensional system of N_e electrons at zero temperature the electron-phonon interaction results in a self-consistent Peierls periodic chain deformation with the period determined by the relation (5.11). This relation is usually called the Peierls relation. Deforming the chain, the electrons create for themselves a single-gap periodic potential (3.11) in which the second parameter ω' is given by (5.12). The energy gap, a single one in the electron spectrum, separates the occupied states from the empty sublevels. The ground-state energy then gets decreased extremely.

The lattice modulation is associated with that of the electron density (2.15)

$$\rho_1(x) = \frac{1}{\kappa} \left[-\frac{\eta'}{\omega'} - \wp(x + \omega') \right]. \quad (5.14)$$

The integration of (5.14) over one period 2ω

$$\int_x^{x+2\omega} \rho_1(x') dx' = 2$$

reveals that there are two electrons per each CDW period at zero temperature.

Calculation of the quantum-mechanical average of the

electron momentum (2.20) gives the known relation $\bar{p}_v = (m/\hbar)[d\mathcal{E}_v(k)/dk]$. Hence, there is no quantum-mechanical contribution of the electrons to the total momentum (2.18). In moving reference frame the CDW state represents the Peierls dielectric. In laboratory reference frame the transition to which is given by the unity transformation

$$T(\mathcal{P}) = \exp \left[-i \frac{V\mathcal{P}}{\hbar} t \right]$$

the wave function (2.5) describes the Fröhlich state with the total momentum (2.18) and the electric current $j = eN_e V$ generated by the motion of CDW as the entity along the chain with velocity $V = dE/dP$.

VI. DISCUSSION OF RESULTS

To analyze the formulas obtained describing the CDW state it is convenient to rewrite them via the Jacobi θ functions.^{13,14} So, in the laboratory reference frame the electron density distribution along the chain (5.14) can be written as

$$\rho_1 = \frac{1}{\kappa} \frac{d^2}{dx^2} \ln \bar{\theta}_2(v) = \sum_{n=-\infty}^{\infty} \frac{\kappa}{\cosh^2 \left[\kappa \left(x - Vt - \frac{\pi}{k_F} n \right) \right]} \quad (6.1a)$$

$$= \frac{n_e}{a} + \frac{1}{\kappa} \frac{d^2}{dx^2} \ln \theta_4(v) = \frac{n_e}{a} \left\{ 1 + \frac{4\pi k_F}{\kappa} \sum_{n=1}^{\infty} \frac{nq^n}{1-q^{2n}} \cos[2k_F n (x - Vt)] \right\}. \quad (6.1b)$$

For the total momentum (2.18) and the energy (2.19) we get the following equations

$$P = V(m + m_1)N_e, \quad (6.2)$$

$$E = \left\{ -\frac{\hbar^2 k_F^2}{6m} \frac{\theta_1'''}{\pi^2 \theta_1'} - \frac{\hbar^2 k_F \kappa}{\pi m} + \frac{1}{2} (m + 2m_1) V^2 \right\} N_e \quad (6.3a)$$

$$= \left\{ \frac{\hbar^2 \kappa^2}{6m} \frac{\bar{\theta}_1'''}{\pi^2 \bar{\theta}_1'} + \frac{1}{2} (m + 2m_1) V^2 \right\} N_e, \quad (6.3b)$$

where

$$m_1 = \frac{2\hbar^2 k_F \kappa}{\pi m V_s^2 (1-s^2)} \left\{ 1 + \frac{\pi^2 k_F^2}{72\kappa^2} \left[\theta_2^8 + \theta_3^8 + \theta_4^8 - 2 \left(\frac{\theta_1'''}{\pi^2 \theta_1'} \right)^2 \right] \right\} \quad (6.4a)$$

$$= \frac{2\hbar^2 \kappa^2}{3m V_s^2 (1-s^2)} \left\{ -\frac{\bar{\theta}_1'''}{\pi^2 \bar{\theta}_1'} + \frac{\pi \kappa}{24k_F} \left[\bar{\theta}_2^8 + \bar{\theta}_3^8 + \bar{\theta}_4^8 - 2 \left(\frac{\bar{\theta}_1'''}{\pi^2 \bar{\theta}_1'} \right)^2 \right] \right\} \quad (6.4b)$$

characterizes the increase of CDW effective mass per electron due to the deformation.

The electron spectrum in the CDW state is characterized by the energy-band position (4.9) with allowance for (5.10). For the filled band width we find

$$\mathcal{L} = \mathcal{E}_2 - \mathcal{E}_1 = \frac{\hbar^2}{2m} (e_1 - e_2) = E_F \theta_4^4 = \frac{\hbar^2 \kappa^2}{2m} \bar{\theta}_2^4. \quad (6.5)$$

The energy gap separating the occupied states from emp-

ty sublevels will then be as follows:

$$\Delta = \mathcal{E}_3 - \mathcal{E}_2 = \frac{\hbar^2}{2m} (e_2 - e_3) = E_F \theta_2^4 = \frac{\hbar^2 \kappa^2}{2m} \bar{\theta}_4^4. \quad (6.6)$$

Here $E_F = \hbar^2 k_F^2 / 2m$ is the Fermi energy of free electrons.

In this formula $\theta_j(v) = \theta_j(v, q)$, $\theta_j = \theta_j(O, q)$ are the Jacobi θ functions ($j=1,2,3,4$) with the parameter $q = \exp(i\pi\tau)$, $\tau = \omega'/\omega$ and $\bar{\theta}_j(\dot{v}) = \theta_j(\dot{v}, \dot{q})$, $\bar{\theta}_j = \theta_j(O, \dot{q})$ are the θ functions with the parameter $\dot{q} = \exp(i\pi\dot{\tau})$ con-

nected with the functions $\theta_j(v, q)$ by the Jacobi imaginary transformation¹⁴ under which $\dot{v} = v/\tau$, $\dot{\tau} = -1/\tau$. According to (5.11) and (5.12) we have for the CDW states

$$v = \frac{x - Vt}{2\omega} = \frac{k_F}{\pi}(x - Vt), \quad q = \exp\left[-\pi \frac{k_F}{\kappa}\right], \quad (6.7a)$$

$$\dot{v} = -i \frac{\kappa}{\pi}(x - Vt), \quad \dot{q} = \exp\left[-\pi \frac{\kappa}{k_F}\right]. \quad (6.7b)$$

If the inequality

$$\frac{k_F}{\kappa} = \frac{\pi \hbar^2 \omega n_e (1 - s^2)}{8mg^2 a^2} > 1 \quad (6.8)$$

is satisfied, then, according to (6.7a), the Jacobi parameter q is the small parameter. In this case it is expedient to make use of the equations written via $\theta_j(v, q)$. The inequality (6.8) is satisfied at small velocity of CDW when $s^2 = V^2/V_s^2 \ll 1$ and at high enough concentration of the electrons. At certain finite value n_e the condition (6.8) can be called the condition of weak electron-phonon coupling.

According to (6.1a) the CDW represents a set of periodically distributed solitons. If the inequality (6.8) is satisfied the solitons are strongly overlapped and it is more convenient to use the expression (6.1b) for ρ_1 . If we neglect the terms of q^2 order in expansion (6.1b) we get the Fröhlich approximation.¹ For the filled band width (6.5) and the energy gap (6.6) we then have

$$\mathcal{L} = E_F(1 - 8e^{-\pi k_F/\kappa}), \quad \Delta = 16E_F e^{-\pi k_F/\kappa}. \quad (6.9)$$

In the same approximation we get from (6.3a) and (6.4a) the CDW energy and the value m_1

$$E = \left\{ \frac{1}{3} E_F - \frac{2g^2 n_e}{w} + \frac{1}{2} (m + m_1) V^2 + O(q^2) \right\} N_e, \quad (6.10)$$

$$m_1 = \frac{4g^2 n_e}{w V_s^2} + O(q^2).$$

Consider now the case when there holds the inequality, inverse to that of (6.8)

$$\frac{\kappa}{k_F} = \frac{8mg^2 a^2}{\pi \hbar^2 \omega n_e (1 - s^2)} > 1. \quad (6.11)$$

Under weak electron-phonon coupling, i.e., when the inequality (6.8) is satisfied at small velocities, $V \approx 0$, the condition (6.11) corresponds to a large enough velocity of CDW motion along the chain so that

$$V^2 > \left[1 - \frac{8mg^2 a^2}{\pi \hbar^2 \omega n_e} \right] V_s^2.$$

In the general case the inequality (6.11) is satisfied at a small enough density of the electrons or relatively strong electron-phonon coupling. In this case the Jacobi parameter \dot{q} (6.7b) becomes the small parameter and it is expedient to use the expression written in terms of the transformed θ functions $\bar{\theta}_j(\dot{v}) = \theta_j(\dot{v}, \dot{q})$.

When the condition (6.11) is satisfied the distance

π/k_F between the solitons (more exactly bisolitons) in the CDW will be larger than the size of the bisoliton π/κ . The momentum (6.2) and the energy (6.3b) of CDW will then be equal to

$$P = P_{bs}(V) \times \frac{1}{2} N_e, \quad E = E_{bs}(V) \times \frac{1}{2} N_e \quad (6.12)$$

and are correspondingly the sums of the momenta

$$P_{bs}(V) = \left[2m + \frac{4\hbar^2 \kappa_0^2}{3m V_s^2 (1 - s^2)^3} \right] V \quad (6.13)$$

and of the energies

$$E_{bs}(V) = -\frac{\hbar^2 \kappa_0^2}{3m} + \frac{1}{2} \left[2m + \frac{4\hbar^2 \kappa_0^2 (1 + \frac{3}{2}s^2 - \frac{1}{4}s^4)}{3m V_s^2 (1 - s^2)^3} \right] V^2 \quad (6.14)$$

of $N_e/2$ noninteracting bisolitons considered in Ref. 6. For the occupied band width (6.5) and the energy gap (6.6) we then get

$$\mathcal{L} = \frac{8\hbar^2 \kappa^2}{m} e^{-\pi(\kappa/k_F)}, \quad \Delta = \frac{\hbar^2 \kappa^2}{2m} (1 - 8e^{-\pi(\kappa/k_F)}), \quad (6.15)$$

i.e., in the case the energy gap exceeds much the width of the filled state band.

As it was mentioned, the Fröhlich sliding-mode conduction which results from depinning of the CDW is widely investigated experimentally (see, for example, reviews by Grüner³). Nonlinear conductivity region was observed above pinning threshold, and the spectral analysis of the current indicates the presence of its oscillations (narrow-band noise) with fundamental frequency ν , proportional to the average current, and several harmonics $\nu_n = \nu n$ with slowly decreasing intensities.

The current flowing through the chain cross section $x = x_0$ can be written in the form

$$j_{CDW}(t) = eV\rho_1(x_0, t).$$

Taking into account Eq. (6.1b), one finds

$$j_{CDW}(t) = \langle j_{CDW} \rangle + 2 \sum_{n=1}^{\infty} c_n \cos(2\pi n \nu t - \alpha_n), \quad (6.16)$$

$$\alpha_n = 2k_F x_0 n.$$

This expression represents the Fourier cosine series and can be used for harmonic analysis of the current, resulting from the CDW motion. As it follows, the current consists of the constant term

$$\langle j_{CDW} \rangle = \frac{en_e}{a} V \quad (6.17)$$

and oscillating term, which is characterized by the fundamental frequency

$$\nu = \frac{k_F}{\pi} V = \frac{k_F a}{\pi n_e e} \langle j_{CDW} \rangle = \frac{1}{2e} \langle j_{CDW} \rangle \quad (6.18)$$

and its harmonics $\nu_n = \nu n$ with amplitudes, decreasing with n

$$C_n = \frac{4\pi k_F}{\kappa} \langle j_{\text{CDW}} \rangle \frac{n}{\sinh \left[\frac{\pi k_F n}{\kappa} \right]} . \quad (6.19)$$

The possibility of such NBN interpretation has also been pointed out by Belokolos.⁴

It is to be noted that the CDW velocity V cannot exceed the sound velocity V_s for at V approaching V_s the CDW energy E and momentum P increase infinitely. As a result the average current (6.17) has to be less than the value $en_e V_s/a$. On this reason the dc I - V characteristics

has to show the tendency of current saturation. It is not improbable that this circumstance is one of reasons for the nonlinear character of sliding-mode conductivity.

In conclusion we note that the continuum approximation used will be justified only when

$$\frac{k_F a}{\pi} < 1 \text{ and } \frac{\kappa a}{\pi} < 1 .$$

This imposes constraints on the electron concentration in the chain, the electron-phonon interaction constant, and also on the CDW motion velocity which cannot be too close to that of sound.

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