# Sound and charge-density wave in the discrete Peierls model

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Small oscillations are considered in the exactly integrable [Sov. Phys. JETP **56**, 212 (1982)] discrete Peierls model. In the exactly integrable model, where there is no pinning, the spectrum has two zero-gap Goldstone modes—sound and a charge-density wave. The stability of multiband stationary states is studied.

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## 1. INTRODUCTION

We have recently constucted and solved an exactly integrable one-dimensional Peierls-transition model.[1] It comprises a special generalization of the known discrete model of Su, Schrieffer, and Heeger.[2] The system energy consists of the energy $\Sigma E$ of the electrons in the self-consistent field of the ions and of the potential energy $W(x_n)$ of the atoms

$$\mathcal{H}=\sum_{E<\mu} E+W. \tag{1.1}$$

The kinetic energy of atoms was omitted (mass $M\to\infty$). In our model the electron spectrum is defined by the equation

$$c_n\psi_{n+1}+c_{n-1}\psi_{n-1}=E\psi_n, \tag{1.2}$$

$$c_n=\exp\,(x_n-x_{n+1}),$$

and the potential energy is chosen in the form of a finite or infinite number of so-called integrals of the Langmuir chain

$$W=-PI_0+\sum_{k=1}^{l}\varkappa_k I_{2k},$$

$$I_0=N^{-1}\sum_n \ln c_n,\quad I_2=N^{-1}\sum_n c_n^2, \tag{1.3}$$

$$I_4=N^{-1}\sum_n\left(c_n^2c_{n-1}^2+\frac{1}{2}c_n^4\right),\ldots,$$

where $P$ is the pressure. We found in Ref. 1 all the extremals of (1.1):

$$\delta\mathcal{H}/\delta c_n=0 \tag{1.4}$$

and showed that they are the so-called finite-band potentials of Eq. (1.2), where the number $q$ of the forbidden bands does not exceed $4l-2$, where $l$ is the number of integrals in (1.3). In particular, for $l=1$ and for an arbitrary number $\rho$ (other than 1 or 2) of electrons per atom ($0<\rho<2$) there is only one two-band extremal (Fig. 1). The structure is always (i.e., at all $l$) symmetric about $E=0$ (see Ref. 1). The total number of states in all the bands is equal to 2; the number of states in the central band of Fig. 1 is equal to $|\rho-1|$. The chemical potential lies in the lower forbidden band at $\rho<1$ and in the upper at $\rho>1$ (Ref. 1, see also Sec. 3).

In view of the exact integrability of (1.4), a number $[\frac{1}{2}(q+1)]$ (see Sec. 2 below) of charge-density waves (CDW) can move in the system relative to the atomic lattice and relative to one another without changing the energy of the system. We must add ordinary sound to these Goldstone bosons (CDW). If a term that upsets the exact integrability of the problem (1.4) is included in the potential energy (1.3), all the CDW lose their freedom to move (pinning sets in)[3] and only one of the Goldstone bosons remains—ordinary sound.

In this paper we take account of the fact that the mass $M$ of the atoms is finite, and add to $\mathcal{H}$ their kinetic energy:

$$\mathcal{H}\to\mathcal{H}+\frac{1}{2}N^{-1}\sum_n M\dot{x}_n^2.$$

Within the framework of the adiabatic approximation $m/M\ll 1$ ($m$ is the electron mass) we confine ourselves to small oscillations about the equilibrium position (1.4) and obtain the spectrum $\varepsilon(k)$ of the linear problem

$$N^{-1}\sum_n\frac{1}{2}M(\delta\dot{x}_n)^2+\delta^2\mathcal{H}. \tag{1.5}$$

We note the characteristic phenomenon of dynamic pinning, which is due to the fact that the time-dependent problem (15) is no longer exactly integrable even if $\mathcal{H}$ is exactly integrable in the static sense. Therefore allowance for the energy of the zero-point oscillations

$$\frac{1}{2}\hbar\sum\varepsilon(k)$$

leads to pinning and, in particular, to a dependence of the "devel's staircase" type on the number of electrons (cf. Ref. 3).

The plan of the paper is the following. In Sec. 3 we calculate the second (i.e., quadratic in $\delta x_n$) variation $\delta^2\mathcal{H}$, and in Sec. 4 we obtain the oscillation spectrum for the integrable case (1.1)–(1.3). In Sec. 5, on the basis of the formula obtained in Sec. 3 for $\delta^2\mathcal{H}$, we investigate the stability of the multiband extremals.

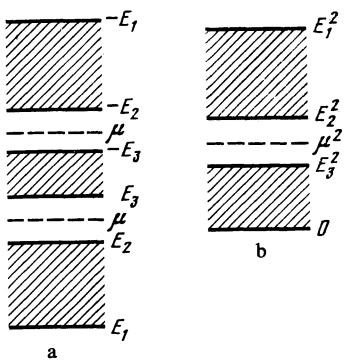


FIG. 1.

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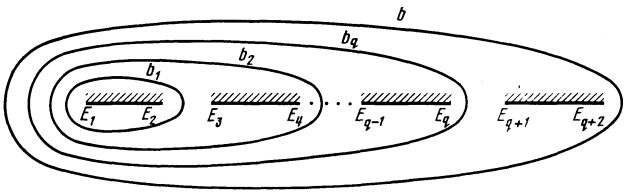


FIG. 2.

We shall need in our calculations some additional mathematical data that could be dispensed with in Refs. 1 and 3. These are briefly expounded in Sec. 2.

## 2. MULTIDIMENSIONAL RIEMANN THETA FUNCTIONS AND FINITE-BAND POTENTIALS OF EQ. (1.2)

An extensive mathematical literature is devoted to the determination of the finite-band potentials of a number of equations, e.g., the Schrödinger equation or its discrete analog (1.2). The necessary information can be found in the known Ref. 4. The wave functions and potentials of Eq. (1.2) for $N$ particles on a ring are finite-band and are completely determined by specifying the beginnings $E_1, E_3, \ldots E_{2q+1}$ and the ends $E_2, \ldots, E_{2q+2}$ of the allowed bands, as well as by specifying the points $E_{2i} \leqslant \gamma_i \leqslant E_{2i+1}$ of the spectrum of the operator (1.2) in the problem with zero boundary conditions $\psi_0 = \psi_N = 0$. We note that the functional (1.1) itself depends only on $E_i$. The leeway in the choice of $\gamma_i$ at fixed $E_i$ is responsible for the already mentioned zero modes of $\mathscr{H}$. Such a spectrum, which has $q$ forbidden bands, is customarily called $q$-band (see, in particular, §4 in Ref. 1). The band boundaries define a hyperelliptic Riemann surface

$$y^2 = R(E), \quad R(E) = \prod_{k=1}^{2q+2} (E - E_k). \tag{2.1}$$

The latter defines in turn a Riemann $\theta$ function of $q$ complex variables $v_1, \ldots, v_q$. In terms of this function it is easy to express the wave function $\psi_n$ and the potentials $c_n$.

The method of constructing $\theta$ functions for the surface $\Gamma$ (2.1) is described in detail in the already mentioned book,[4] or as applied to the discrete equation (1.2) on a paper by one of us.[5] Much information on $\theta$ functions can be found in Dubrovin's review.[6] Here we only list the results, and refer the reader for proofs in, e.g., Refs. 4–6.

The Riemann surface $\Gamma$ of the function (2.1) is a surface of kind $q$ in a two-dimensional complex space $(y, E)$ (the surface $\Gamma$ is equivalent to a sphere with $q$ knobs). It obviously corresponds to the product of $q+1$ cuts along the allowed bands (Fig. 2). A complex surface of kind $q$ has (see, e.g., Ref. 4) $2q$ independent cycles. The cycles $a_1, \ldots, a_q$ go over the forbidden bands (Fig. 3), and the cycles $b_1, \ldots, b_q$ are shown in Fig. 3. The projection of the cycles $b_k$ on the physical energy plane $E$ is shown in Fig. 2; they encircle respectively $1, 2, \ldots, q$ allowed bands. The function $R^{1/2}(E)$ becomes single-valued on the surface $\Gamma$.

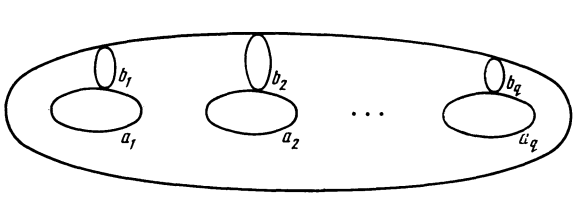


FIG. 3.

We define $q$ holomorphic differentials $\omega_k$ on $\Gamma$. They are given by

$$\omega_k = \frac{Q_k(E)}{R^{1/2}(E)} dE, \tag{2.2}$$

where $Q_k(E)$ are polynomials of degree $q-1$. Their coefficients ($q^2$ in number) are uniquely determined from the $q^2$ conditions

$$\oint_{a_l} \omega_k = \delta_{kl}. \tag{2.3}$$

The integrals of $\omega_k$ over the cycles $b_k$ specify the matrix of the Riemann coefficients

$$B_{kl} = \oint_{b_l} \omega_k. \tag{2.4}$$

It is symmetric and has a positive imaginary part.

We introduce finally the quasimomentum $p$ with the aid of the relation (cf. Ref. 1)

$$idp = (E^q + r_1 E^{q-2} + \ldots) R^{-1/2} dE. \tag{2.5}$$

The coefficients $r_1, \ldots,$ are determined from physically obvious conditions whose meaning is that the number of states in each forbidden band is zero:

$$\oint_{a_k} dp = 0. \tag{2.6}$$

The differential $idp$ is not holomorphic. It has simple poles in the operands of infinite energy $E_\infty^+$ and $E_\infty^-$ on the Riemann surface, with residues $+1$ and $-1$, respectively.

The definition (2.5) of the quasimomentum differs somewhat from the customary one. The quasimomentum $p$ of (2.5) is not referred to an actual Brillouin zone specified by a real lattice period, and is normalized by the condition that the number of states in all the allowed bands be equal to unity. In this case $p > 0$ and runs through values from zero to $\pi$. To verify this, we recall that states in allowed bands are doubly degenerate[1,4] (the obvious $p \to -p$ degeneracy). Therefore the total number of states is

$$\frac{2}{2\pi} \int_{E_1}^{E_{2q+2}} dp = \frac{1}{2\pi} \oint_b dp,$$

where $b$ is a cycle that encloses all the allowed bands (see Fig. 2). The integral with respect to $b$ can be taken along a contour that encloses one infinity on $\Gamma$. It follows then directly from (2.5) that

$$\frac{1}{\pi} \int_{E_1}^{E_{2q+2}} dp = \operatorname{res}_{+\infty} ip = 1.$$

The number $\rho$ of occupied states (the number of electrons per atom) is given, with allowance for the spin, by

$$\frac{2}{\pi} \int_{E_1}^{\mu} dp = \rho = \frac{1}{\pi} \oint_{b_\mu} dp, \tag{2.6'}$$

where the cycle $b_\mu$ encloses all the filled bands.

We are now in a position to define the Bloch wave function $\psi_n(E)$ as a single-valued function of the energy $E$ [or of $\gamma(E)$] on the Riemann surface $\Gamma$ (cf. Refs. 1 and 4–6)). It is for this purpose that one uses the multidimensional $\theta$ functions, which are naturally connected with the Riemann surface of $q$ variables $v_1,\ldots,v_q$. The function $\theta$ is given by

$$\theta(v_1,\ldots,v_q) = \sum_{m_1=-\infty}^{\infty}\cdots\sum_{m_q=-\infty}^{\infty}\exp\left\{\pi i\sum_{k,l=1}^{q}B_{kl}m_km_l+2\pi i\sum_{k=1}^{q}v_km_k\right\}. \tag{2.7}$$

In the case $q=1$ Eq. (2.7) reduces to the standard elliptic function $\theta_3(v,\tau)$ with $\tau=B_{11}$. When speaking of one-dimensional elliptic functions we shall hereafter use, unless otherwise stipulated, the standard notation of the Erdelyi-Bateman tables.[7]

The function (2.7) has periodicity properties that generalize in natural fashion the equations for $\theta_3(v,\tau)$. Namely, when any of the $v_q$ is shifted by unity the function $\theta$ is not changed, but following the shift

$$v_k\to v_k+B_{kl}$$

we have for any fixed $l$

$$\theta(v_k+B_{kl})=\theta(v_k)\exp(-\pi iB_{ll}-2\pi iv_l). \tag{2.8}$$

We introduce finally three different $q$-dimensional vectors. One $\mathbf{A}=\{A_k\}$ depends on the energy $E$ [of the point $\gamma(E)$]

$$A_k(\gamma)=\int_{E_1}^{\gamma}\omega_k, \tag{2.9}$$

and the other two are constant, i.e., independent of the energy $\gamma(E)$, namely $\mathbf{U}$:

$$U_k=\frac{1}{2\pi}\oint_{b_k}dp, \tag{2.10}$$

and $\mathbf{V}=\{V_K\}$. The Bloch function is then given by

$$\psi_n(\gamma)=r_n\exp\left\{in\int_{E_1}^{\gamma}dp\right\}\frac{\theta(\mathbf{A}+n\mathbf{U}+\mathbf{V})}{\theta(\mathbf{A}+\mathbf{V})}. \tag{2.11}$$

As explained in Ref. 1, the products $NU_k$ ($N$ is the number of atoms) are integers, so that the function $\psi_n(\gamma)$ has in accord with the properties of $\theta$ the correct Bloch behavior:

$$\psi_{n+N}(\gamma)\to\psi_n(\gamma)\exp(iNp(\gamma)).$$

The function $\psi_n$ does not change when $\gamma$ encircles any of the cycles $a$ or $b$. On circling along $a_l$ we have

$$\psi_n\to\psi_n\exp\left\{in\oint_{a_l}dp\right\}\theta(\mathbf{A}+\mathbf{V})\theta\left(A_k+nU_k+V_k+\oint_{a_l}\omega_k\right)\times\left[\theta(\mathbf{A}+n\mathbf{U}+\mathbf{V})\left(A_k+V_k+\oint_{a_l}\omega_k\right)\right]^{-1},$$

which coincides with $\psi_n$ by virtue of (2.3) and (2.6). On circling along $b_l$,

$$\psi_n\to\psi_n\exp\left\{in\oint_{b_l}dp\right\}\theta(\mathbf{A}+\mathbf{V})\theta(A_k+B_{kl}+nU_k+V_k)\times[\theta(\mathbf{A}+n\mathbf{U}+\mathbf{V})\theta(A_k+B_{kl}+V_k)]^{-1}$$

$$=\psi_n\exp\left\{in\oint_{b_l}dp-2\pi inU_l\right\},$$

which coincides with $\psi_n$ by virtue of (2.10).

To find the hop-over integrals, meaning the potentials $c_n=\exp(x_n-x_{n+1})$, and the displacements $x_n$ it suffices to consider the behavior of the wave functions $\psi_n$ at infinite energy. It is known (see, e.g., Refs. 1, 4, 5) that at a certain renormalization we have

$$\psi_n\to\exp(\pm x_n)E^{\pm n},$$

when $E$ tends to the upper ( + ) or lower ( − ) transform of infinity on the Riemann surface. Therefore

$$\exp(2x_n)=E^{-2n}\psi_n(E+)/\psi_n(E-),\quad E\to\infty$$

with $\psi_n$ from (2.11). Recalling also the formula for the quasimomentum (Refs. 1, 4, 5)

$$ip(E\pm)=\pm(\ln E-I_0-I_2E^2-\ldots),$$

we obtain

$$\exp(2x_n)=\exp(-2nI_0)\theta(-A_{k0}+V_k)\theta(A_{k0}+nU_k+V_k)\times[\theta(A_{k0}+V_k)\theta(-A_{k0}+nU_k+V_k)]^{-1},$$

where $\pm A_{k0}$ are the transforms of the functions $A_k$ at both infinities. Using Riemann's known bilinear relations (see, e.g., Ref. 6)

$$A_{k0}={}^1/_2-U_k, \tag{2.12}$$

we obtain ultimately

$$\exp(2x_n)=\exp(-2nI_0)\theta(U_k+\Phi_k)\theta((n-1)U_k+\Phi_k)\times[\theta(-U_k+\Phi_k)\theta(n+1)U_k+\Phi_k)]^{-1}, \tag{2.13}$$

where $\Phi_k=V_k+\frac{1}{2}$ is the set of $q$ constants that constitute the "coordinates" of $q$ charge-density waves.

For the Schrödinger equation (1.2), the spectrum is symmetric:

$$E\to-E,\qquad \psi_n\to(-)^n\psi_n \tag{2.14}$$

(see Fig. 1). Therefore the matrix $B_{kl}$ has an additional symmetry, which enabled us earlier[1] to solve the problem and express the quantities of physical interest, including the displacement $x_n$ and the charge density $\psi_n^2$, in terms of ordinary elliptic functions without resorting directly to the general-theory results presented here. The calculations that follow for the oscillation spectrum are essentially based on Eq. (2.11).

## 3. SECOND VARIATION OF THE ENERGY

We confine ourselves here to the physically most interesting three-band case of Fig. 1, and defer the discussion of the multiband situation to Sec. 5.

At arbitrarily small variations $\delta x_n$ of the ion positions (and $\delta c_n$ of the potentials) the spectrum of Eq. (1.2) is no longer three-band. New gaps appear in the allowed bands, and their number can in principle be arbitrarily large (of the order of the number $N$ of the atoms). From the spectrum-formation picture described earlier[1] (see in particular Fig. 3 of Ref. 1) it is clear that at infinitely small variations no new narrow allowed bands will appear in the initial forbidden

bands in Fig. 1. The displacements of the boundaries of the old bands $E_1, E_2, E_3$ in the limit as $N\to\infty$, which are possible in principle, are of course immaterial.

It turns out that there is a simple formula that expresses the second variation in terms of the squares of the widths $(\delta e_j)^2$ of the new gaps ($j$ is the number of the new forbidden band). It was recently obtained by one of us[5] for the previously considered[1] model II. Here we describe its derivation for the problem (1.1)–(1.4) (model I of Ref. 1).

We write the total energy in the form

$$\mathcal{H}=\frac{1}{\pi}\oint_{b_\mu} E\,dp-PI_0+\varkappa I_2. \tag{3.1}$$

$R(E)$ should be chosen to be

$$R^2=(E^2-E_1^2)(E^2-E_2^2)(E^2-E_3^2). \tag{3.2}$$

For the quasimomentum we have the formula[1]

$$i\,dp=(E^2+C)R^{-1/2}(E)\,dE \tag{3.3}$$

and $C$ from (4.23) of Ref. 1. We recall also that at the energy $E$ that tends to the upper infinity we have[1]

$$ip=\ln E-I_0-I_2E^{-2}-I_4E^{-4}-\dots\ . \tag{3.4}$$

The $E\to -E$ symmetry allows us to operate with the picture of the spectrum using the variables $E^2$ (Fig. 1b). The opening-up of new $K<N$ gaps $\delta e_j^2$ at the points $e_j^2$ (Fig. 4), where $e_{j\pm}^2=e_j^2\pm\frac{1}{2}\delta e_j^2$, is described by the obvious formula for the quasimomentum:

$$i\,dp=Q_{2K+2}(E)\left[R(E)\prod_{j=1}^{K}(E^2-e_{j+}^2)(E^2-e_{j-}^2)\right]^{-1/2}dE, \tag{3.5}$$

where $Q_{2K+2}$ is a polynomial of degree $2K+2$ with coefficients determined by the conditions (2.6) for all cycles $a_j$ on Fig. 4. Variation of the $e_{j\pm}^2$ likewise does not alter the integrals along the cycles $b_j$, since[1] they are rational numbers. Therefore

$$\delta\oint_{a_j} dp=\delta\oint_{b_j} dp=\delta\oint_{b_\mu} dp=0. \tag{3.6}$$

In addition, the polynomial $Q_{2k+2}$ should be such that when one of the gaps collapses, namely $\delta e_j^2=0$, any trace of its existence, i.e., the point $e_j^2$, would vanish from Eq. (3.5):

$$Q_{2K+2}\to(E^2-e_j^2)Q_{2K},\qquad \delta e_j^2\to 0. \tag{3.7}$$

Expanding (3.5) up to terms of second order in $\delta e_j^2$ we obtain

$$i\delta dp=\tilde{Q}_{4K+2}R^{-1/2}(E)\prod_{j=1}^{K}(E^2-e_j^2)^{-2}, \tag{3.8}$$

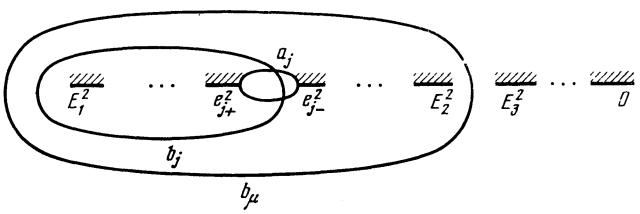


FIG. 4.

where the coefficients of the polynomial $\tilde{Q}_{4K+2}$ are certain expressions that are quadratic in $\delta e_j^2$. By virtue of the conditions (3.6), the residues $\delta dp$ at the points $e_j^2$ are zero. Moreover, since the integrals of $\delta dp$ over all the cycles $a_j$ and $b_j$ vanish, the integral of $\delta dp$ is uniquely defined:

$$\delta p=\int_{E_1}^{E}\delta dp.$$

It is a meromorphic function with simple poles at the point $e_j$. Its behavior at large $E$ is determined from (3.4):

$$i\delta p=-\delta I_0-E^{-2}\delta I_2-E^{-4}\delta I_4-\dots\ . \tag{3.9}$$

Hence

$$i\delta p=\frac{BE^3+DE}{R^{1/2}(E)}+\frac{E}{R^{1/2}(E)}\sum_j\frac{A_j}{E^2-e_j^2}. \tag{3.10}$$

The coefficients $A_j$, $B$, and $D$ are certain quadratic forms of $\delta e_j^2$. The coefficients $A_j$ can be easily found by differentiating (3.10) with respect to the energy $E$ and comparing the senior-order singularities with (3.8). This yields

$$A_j=-\tfrac{1}{16}e_j^{-2}(e_j^2+C)(\delta e_j^2)^2 \tag{3.11}$$

with $C$ from (3.3). The coefficients $B$ and $D$ contain also mixed terms $\delta e_j^2\delta e_k^2$ and terms linear in $\delta e_j^2$. The coefficients $B$ and $D$, however, make no contribution whatever to the second variation of the energy for the extremals of the functionals (3.1).

The last circumstance follows from the fact that $B$ and $D$ can be expressed with the aid of (3.9) in terms of $\delta I_0$ and $\delta I_2$. Comparison of the constant terms and of the terms of order $E^{-2}$ yields

$$B=-\delta I_0,\quad D-\tfrac{1}{2}Bs_2=-\delta I_2,$$
$$s_2=-E_1^2-E_2^2-E_3^2.$$

The corresponding part of the momentum variation

$$i\delta p=(BE^3+DE)/R^{1/2}(E)$$

has the same structure as the first momentum variation given by Eqs. (4.9) of Ref. 1. Therefore its contribution to the energy (3.1) is cancelled by $-P\delta I_0+\varkappa\delta I_2$ by virtue of the conditions for the consistency on the extremals (4.20) and (4.21) of Ref. 1. Only the terms of (3.10) contribute to the variation. Taking (3.11) into account, we can write the final formula

$$\delta^2\mathcal{H}=\sum_j\mu_j(\delta e_j^2)^2,$$
$$\mu_j=\mu(e_j^2)=\frac{1}{8\pi i}\frac{e_j^2+C}{e_j^2}\int_{E_1}^{\mu}\frac{E\,dE}{R^{1/2}(E)(E^2-e_j^2)}. \tag{3.12}$$

The constant $C$ of (3.3) was defined by Eqs. (5.20) in Ref. 1.

Equation (3.12) and its generalization to the multiband case, considered in Sec. 5 below, are extremely convenient for the investigation of the stability of the extremal. However, its diagonal form notwithstanding, its "eigenvalues" $j$ do not yield directly the lattice vibration frequencies. The point is that in the space of the atom displacements $\delta x_n$, where the kinetic energy (1.5) is specified, the "eigenvectors"

$\delta e_j^2$ are not orthogonal at all (besides the obvious double degeneracy). To find the frequencies it is necessary also to express $\delta e_j^2$ in terms of $\delta x_n$.

## 4. FREQUENCIES OF LATTICE VIBRATIONS

Let us calculate the displacements that correspond to opening-up of exactly one gap $\delta e_j^2$ against the unperturbed background in Fig. 1b. We use here explicitly the symmetry of the spectrum (2.13), by virtue of which the squared wave function $\psi_n^2$ depends only on $E^2$. In terms of $E^2$ and $\psi^2$ we can literally repeat everything said in Sec. 2. We put $E^2=\lambda$ and furthermore

$$\delta e_j^2=\delta\lambda_j, \quad E_1^2=\Lambda_1, \quad E_2^2=\Lambda_2, \quad E_3^2=\Lambda_3.$$

For the holomorphic differentials and for quasimomentum on the surface $\lambda$ we use the capital letters $\Omega_k$ and $P$, respectively. The cuts and the cycles on the $\lambda$ plane are shown in Fig. 5, where $\lambda_\pm=\lambda_0\pm\frac{1}{2}\delta\lambda$. The quasimomentum $P$ is given (at $\delta\lambda=0$) by the formula

$$iP=\int_{\Lambda_1}^{\lambda}\frac{\lambda+C}{[\lambda R(\lambda)]^{1/2}}\,d\lambda, \tag{4.1}$$

where $C$ is the same constant as in (3.3) and $R(\lambda)$ is $R(E)$ from (3.2) but expressed in terms of $\lambda$ and $\Lambda$. It is clear that $P=2p$ (but $0<P<\pi$).

In accord with the exposition in Sec. 2 we have

$$\psi_n^2(\lambda)=r_n\exp\left\{in\int_{\Lambda_1}^{\lambda}dP\right\}\theta^2(A_k(\lambda)+U_kn-V_k)/\theta^2(A_k(\lambda)-V_k). \tag{4.2}$$

Here $\theta$ is the two-dimensional theta funtion ($k=1,2$) corresponding to the Riemann surface of Fig. 5; $A_k$, $P$, and the matrix $B_{kl}$ are determined by the equations of Sec. 2 with the substitution $R(E)\to\lambda R(\lambda)$, and

$$U_k=\frac{1}{4\pi}\oint_{b_k}dP=\frac{1}{2\pi}\oint_{b_k}dp. \tag{4.3}$$

Repeating the arguments that have led to (2.13), we get

$$\exp(4x_n)=\exp(-4nI_0)\,\theta^2(U_k+\Phi_k)\,\theta^2((n-1)U_k+\Phi_k)\times[\theta^2(-U_k+\Phi_k)\,\theta^2((n+1)U_k+\Phi_k)]^{-1}, \tag{4.4}$$

whence we get for small displacements $\delta x_n$ (orthogonal to the constant displacement $\delta x_n=\text{const}$)

$$2\delta x_n=\delta\theta((n-1)U_k+\Phi_k)/\theta((n-1)U_k+\Phi_k)-\delta\theta((n+1)U_k+\Phi_k)/\theta((n+1)U_k+\Phi_k). \tag{4.5}$$

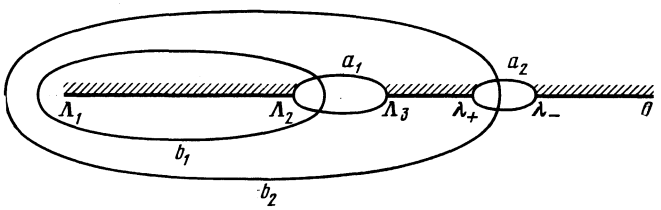


FIG. 5.

In particular, for an equilibrium phason with $\delta\lambda=0$ the theta function is one-dimensional, $U=\rho/2$, and the variation in (4.5) is the variation of the phase $\Phi$. Therefore $\delta x_{\text{ph}}\sim u_{n\,\text{ph}}\delta\Phi$,

$$u_{n\Phi}=\theta_3'(\tfrac{1}{2}\rho(n-1)+\Phi)/\theta_3(\tfrac{1}{2}\rho(n-1)+\Phi)-\theta_3'(\tfrac{1}{2}\rho(n+1)+\Phi)/\theta_3(\tfrac{1}{2}\rho(n+1)+\Phi). \tag{4.6}$$

We are interested in the terms $\sim\delta\lambda$ in the displacement (4.5) as the width $\delta\lambda$ of the additional band tends to zero. These displacements are determined by the limiting behavior the matrix $B_{kl}$ defined in accord with the rules of Sec. 2 and of the vector $U_k$ from (4.3), accurate to $\delta\lambda$.

The unperturbed value of the differential $\Omega_1$ (see Fig. 5) is

$$\Omega_1^{(0)}\equiv\Omega=\frac{d\lambda}{(\lambda R(\lambda))^{1/2}}\Big/\int_{\Lambda_2}^{\Lambda_3}\frac{d\lambda}{(\lambda R(\lambda))^{1/2}}; \tag{4.7}$$

and the unperturbed

$$B_{11}^{(0)}\equiv\tau=\int_{\Lambda_1}^{\Lambda_2}\frac{d\lambda}{(\lambda R)^{1/2}}\Big/\int_{\Lambda_2}\frac{d\lambda}{(\lambda R)^{1/2}}. \tag{4.8}$$

We denote the latter $\tau$ in accord with the remarks made in Sec. 2. The quantity $\tau$ is, e.g., a standard parameter of the function $\theta_3$ in (4.6). Its value was calculated in Ref. 1.

With accuracy linear in $\delta\lambda$, the differential $\Omega_1$ does not change:

$$\Omega_1=\Omega+O(\delta\lambda^2).$$

The same holds, of course, also for $B_{11}$:

$$B_{11}=\tau+O(\delta\lambda)^2,$$

and for $B_{12}$ we have correspondingly

$$B_{12}=2\int_{\Lambda_1}^{\lambda_0}\Omega+O(\delta\lambda).$$

We can also write

$$B_{12}=2A(\lambda_0)\equiv2\alpha, \tag{4.9}$$

where $A(\lambda)$, according to the definitions of Sec. 2, is the limiting value of the component $A_1^{(0)}(\lambda)$ of the vector $A_k$:

$$A(\lambda)=\int_{\Lambda_1}^{\lambda}\Omega=\int_{\Lambda_1}^{\lambda}\frac{d\lambda}{(\lambda R)^{1/2}}\Big/2\int_{\Lambda_2}^{\Lambda_3}\frac{d\lambda}{(\lambda R)^{1/2}}. \tag{4.10}$$

It is convenient to use for the subsequent calculations the elliptic parametrization used earlier in Ref. 1. In the first parametrization (Sec. 5 of Ref. 1) we introduce the variable

$$z_1=\frac{1}{2}\int_{\Lambda_1}^{\lambda}\frac{d\lambda}{(\lambda R)^{1/2}}$$

and everything is expressed in terms of the Weierstrass elliptic functions $\wp(z_1)$, $\zeta(z_1)$, $\sigma(z_1)$ with periods $2\omega_1$ and $2\omega_1'$, shown in Fig. 6a of Ref. 1. In the second parametrization we use Weierstrass functions of

$$z_2=\frac{1}{2}\int_{\Lambda_1}^{\lambda}\frac{d\lambda}{R^{1/2}}$$

with periods $2\omega_2$ and $2\omega_2'$, shown in Fig. 6b in Ref. 1. All the calculations are perfectly analogous to those of Sec. 5 in Ref.

1, therefore we shall as a rule write down the answers directly.

In the first parametrization

$$\omega_1=\frac{1}{2}\int_{\Lambda_1}^{\Lambda_2}\frac{d\lambda}{(\lambda R)^{1/2}},\quad \omega_1'=\frac{1}{2}\int_{\Lambda_2}^{\Lambda_3}\frac{d\lambda}{(\lambda R)^{1/2}},$$

$$\Omega(\lambda)=dz_1/2\omega_1',\quad z_1=2\omega_1'A(\lambda),\quad \tau=\omega_1/\omega_1', \tag{4.11}$$

$$\lambda(z_1)=\tfrac{1}{2}[\zeta(z_1+z_{10})-\zeta(z_1-z_{10})]+h.$$

In the formula for $\lambda$ the parameter $z_{10}$ is the transform of the upper infinity on the Riemann surface:

$$z_{10}=2\omega_1'A_0$$

with $Z_0$ from (2.12). The constant $h$ is determined, as in Ref. 1, from the condition $\lambda(\omega_1')=0$.

It remains to calculate the limiting behavior of the holomorphic differential $\Omega_2$. Since its integral with respect to the contracting cycle $a_2$ is finite, the differential $\Omega_2$ is transformed in the limit as $\delta\lambda\to 0$ into the so-called differential of the third kind (see, e.g., Refs. 4 and 6), with residues $\pm 1$ at the transforms of the point $\delta_0$:

$$\Omega_2\approx\frac{1}{2\pi i}\frac{\pm 1}{\lambda-\lambda_0}d\lambda.$$

In the parametrization of $z_1$ we write directly

$$\Omega_2(z_1)=-\frac{1}{2\pi i}[\zeta(z_1+2\omega_1'\alpha)-\zeta(z_1-2\omega_1'\alpha)+h_1]dz_1 \tag{4.12}$$

with $\alpha$ from (4.9).

The constant $h_1$ is obtained from the normalization condition

$$0=\oint_{a_1}\Omega_2=-\frac{1}{2\pi i}\int_0^{2\omega_1'}[\zeta(z_1+2\omega_1'\alpha)-\zeta(z_1-2\omega_1'\alpha)+h_1]dz_1.$$

This yields

$$h_1=-4\eta_1'\alpha. \tag{4.13}$$

Finally

$$B_{22}=2\int_{\Lambda_1}^{\lambda_+}\Omega_2=-\frac{1}{\pi i}\int_0^{z_+}[\zeta(z+2\omega_1'\alpha)-\zeta(z-2\omega_1'\alpha)$$
$$-4\eta_1'\alpha]dz=-\frac{1}{\pi i}\left(\ln\frac{\sigma(z_++2\omega_1'\alpha)}{\sigma(2\omega_1'\alpha-z_+)}-4\eta_1'\alpha z_+\right),$$
$$z_+=2\omega_1'A(\lambda_+).$$

We expand the result in terms of the small quantity

$$y=z_+-2\omega_1'\alpha\sim\delta\lambda.$$

We have

$$\pi iB_{22}=\ln\sigma(-y)-\ln\sigma(4\omega_1'\alpha)+8\eta_1'\alpha^2\omega_1'+\dots.$$

On the other hand, according to the definition (4.11)

$$\tfrac{1}{2}\delta\lambda=\lambda(z_+)-\lambda(2\alpha\omega_1')=\tfrac{1}{2}\{\zeta(z_++z_{10})$$
$$-\zeta(z_+-z_{10})-\zeta(2\alpha\omega_1'+z_{10})+\zeta(2\alpha\omega_1'-z_{10})\}$$
$$=\tfrac{1}{2}y[-\wp(2\alpha\omega_1'+z_{10})+\wp(2\alpha\omega_1'-z_{10})]+\dots.$$

Finally

$$\pi iB_{22}=\ln\delta\lambda-\ln[\wp(2\alpha\omega_1'+z_{10})$$
$$-\wp(2\alpha\omega_1'-z_{10})]-\ln\sigma(4\omega_1'\alpha)+8\eta_1'\alpha^2\omega_1'+O(\delta\lambda). \tag{4.14}$$

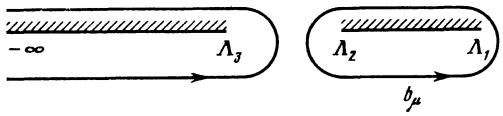


FIG. 6.

When the gap $\delta\lambda$ collapses $iB_{22}\to-\infty$. Therefore in the first-order approximation it suffices to retain in Eq. (2.7) for the $\theta$ function, which is two-dimensional in this case, only terms with $m_2=0,\ \pm 1$. Recalling that $B_{11}=\tau$, we have

$$\theta(v_1,v_2)\approx\theta_3(v_1)+\exp(i\pi B_{22})$$
$$\times\left\{\sum_m\exp[\pi i(\tau m^2+2B_{12}m)+2\pi i(v_1m+v_2)]\right.$$
$$\left.+\sum_m\exp[\pi i(\tau m^2-2B_{12}m)+2\pi i(v_1m-v_2)]\right\}+O(\delta\lambda^2),$$

or

$$\theta(v_1,v_2)\approx\theta_3(v_1)+\exp(\pi iB_{22})[\theta_3(v_1$$
$$+2\alpha)\exp(2\pi iv_2)+\theta_3(v_1-2\alpha)\exp(-2\pi iv_2)]+\dots. \tag{4.15}$$

The increment linear in $\delta\lambda$ to this formula is precisely the same $\delta\theta$ that must be inserted in (4.5) to obtain the perturbation $\delta x_n$ that opens up exactly the only gap of width $\delta\lambda$ at the point $\lambda_0(\theta)$. The lucid form of this increment allows us to determine the general character of the oscillations and calculate the speed of sound in CDW.

In the beginning we did not write out the explicit forms of $v_1$ and $v_2$. We have

$$v_1=nU+\Phi,\quad U=\tfrac{1}{2}\rho,$$

where $\Phi$ is an arbitrary complex number.

Next

$$v_2=nU_2+\varphi,$$

where $\varphi$ is again an arbitrary complex number, and (see (4.3))

$$U=\frac{1}{2\pi}\int_{\Lambda_1}^{\lambda_0}dP=\frac{1}{2\pi}P(\lambda_0)=\frac{1}{2\pi}P(\alpha),$$

where $p(\lambda_0)$ [or $P(\alpha)$] is the value of the quasimomentum at the point where the gap is opened. It is natural to express all the quantities in terms of $P$. This calls for calculation of the functions $\alpha(P)$ and $\lambda_0(P)$.

According to the general properties of the momentum we have

$$idP=[\zeta(z_1+z_{10})-\zeta(z_1-z_{10})+h_2]dz_1.$$

The constant is obtained here from the vanishing of the integral over the cycle $a_1$:

$$0=\int_0^{2\omega_1'}\frac{dP}{dz_1}dz_1.$$

This yields

$$h_2=-2\eta_1'z_{10}/\omega_1'$$

and

$$iP(\alpha)=\ln\frac{\sigma(z_{10}+2\omega_1'\alpha)}{\sigma(z_{10}-2\omega_1'\alpha)}-4\alpha\eta_1'z_{10}. \tag{4.16}$$

Owing to the presence of the complex "phase" $\varphi$ in the equation for $v_2$, the state $\delta x_n$ corresponding to the given $\delta\lambda(P)$ is doubly degenerate. The independent displacements can be chosen to be

$$\delta x_n^{\pm}=\exp(i\pi B_{22}(P))\,u_n^{\pm}(P)\,e^{\pm iPn};$$
$$u_n^{\pm}(P) \tag{4.17}$$
$$=\frac{\theta_3(U(n-1)\pm 2\alpha+\Phi)}{\theta_3(U(n-1)+\Phi)}\,e^{\mp iP}-\frac{\theta_3(U(n+1)\pm 2\alpha+\Phi)}{\theta_3(U(n+1)+\Phi)}\,e^{\pm iP},$$

where $\alpha$ is connected with $P$ by the relation (4.16).

The functions (4.17) have, as expected, an explicit Bloch structure. The lattice period coincides with the period of $\theta_3$, i.e., is equal to the denominator of the irreducible fraction $r$ that specifies the rational number $U=\rho/2$. It is therefore clear beforehand that the spectrum of the vibrations will be determined by an $r\times r$ matrix that connects the vibrations with momenta $P$ that coincide in modulo $2\pi/r$.

Of course, it is possible to transform to an irreducible Brillouin zone with dimension $2\pi/r$ and to an irreducible quasimomentum $0<k<\pi/r$.

In our calculation method the matrix $\delta^2\mathscr{H}$ is diagonal in the basis $\delta x_n^{\pm}(P)$ [or $\delta x_n^{\pm}(\alpha)$], directly diagonal in the representation of the momentum $P$ (or of $\alpha$). Its elements are

$$\operatorname{diag}\delta^2\mathscr{H}=\mu(\alpha)\,\delta\lambda^2/\exp(2\pi i B_{22})\langle|u_n^{\pm}|^2\rangle,$$

where $\langle\ldots\rangle$ is an average over the lattice:

$$\langle\ldots\rangle=N^{-1}\sum_n\ldots$$

Substituting here $B_2$ from (4.14), we get

$$\operatorname{diag}\delta^2\mathscr{H}=\mu(\alpha)\,\sigma^2(4\omega_1'\alpha)\,[\wp(2\alpha\omega_1'+z_{10})-\wp(2\alpha\omega_1'-z_{10})]^2/\exp(16\eta_1'\alpha^2\omega_1')\langle|u_n^{\pm}|^2\rangle, \tag{4.18}$$

where $\mu(\alpha)=\mu(e_j^2)$ from (3.12). On the other hand, a matrix of the form $\Sigma\delta\dot{x}_n^2$ is not diagonal in the basis and breaks up precisely into $r\times r$ blocks. Equations (4.17) and (4.18) reduce in principle the problem of calculating the spectrum to a determination of the eigenvalues of $r\times r$ matrices.

Equations (4.18) permit a rather simple determination of all the zero-gap modes. Clearly, they must be sought among the values of $P$ or $\alpha$ at which $\delta^2\mathscr{H}$ vanishes. It can be seen from (4.18) that there are only four suspicious values:

$$\alpha_1=0,\quad \alpha_2={}^1/_2\tau,\quad \alpha_3={}^1/_2+{}^1/_2\tau,\quad \alpha_4={}^1/_2,$$

accordingly

$$P_1=0,\quad P_2=2\pi U=P_3,\quad P_4=\pi.$$

At these values of $\alpha$ the numerator of (4.18) has a zero of fourth order. On the other hand, according to (4.17) the functions $u^{\pm}$ themselves vanish at these points, and as a result $\delta^2\mathscr{H}$ vanishes quadratically, as was to be expected.

We note also that at the point $\alpha_4$ the variation $\delta^2\mathscr{H}$ remains finite. The point is that the value $\alpha=\frac{1}{2}$ corresponds to an energy $\lambda=0$. Then, according to Eq. (3.12) for $\mu$, this quantity itself becomes infinite like $\sim\lambda^{-2}\sim(\alpha-\frac{1}{2})^{-2}$, canceling out the corresponding zero. The remaining three points correspond respectively to the values $E_1^2(\Lambda_1)$, $E_2^2(\Lambda_2)$, $E_3^2(\Lambda^3)$ on Figs. 4 and 5. This circumstance is in full agreement with our intuitive notion that a zero-gap mode should, in essence, only shift the spectrum boundaries and open up small gaps near $\Lambda_1$, $\Lambda_2$, and $\Lambda_3$.

We note that the momenta $P_2=P_3$ are equal to $\pi\rho$ at $\rho<1$ and are equal to $\pi(2-\rho)$ at $\rho>1$.

It is not difficult to calculate $\delta^2\mathscr{H}$ near the zeros. The corresponding standard calculations with elliptic functions, given in the Appendix, yield

$$\begin{aligned}&\operatorname{diag}_1\delta^2\mathscr{H}=P^2F_1/(1+\varkappa_1^2\langle u_{\rm ph}^2\rangle),\\ &\operatorname{diag}_2\delta^2\mathscr{H}=(P-2\pi U)^2F_2/(1+\varkappa_2^2\langle u_{\rm ph}^2\rangle),\\ &\operatorname{diag}_3\delta^2\mathscr{H}=(P-2\pi U)^2F_3/(1+\varkappa_3^2\langle u_{\rm ph}^2\rangle).\end{aligned} \tag{4.19}$$

In the state 2 the momentum $P<2\pi U$, while in the state 3 it is larger than $2\pi U$. Here $u_{n\rm ph}$ is the phason described by Eq. (4.6). Expressions for $F_\beta$, $\varkappa_\beta$ ($\beta=1,2,3$) are given in the Appendix [Eqs. (A.1)–(A.3) and (A.7)].

If only the zero-gap-mode spectrum is of interest, it suffices to retain from the total $r\times r$ matrix only the $3\times 3$ matrix that connects the three states (4.19). It is then possible to transform the quasi-momentum $k$ and to the reduced Brillouin zone; naturally, in this reduction $P$ and $P-2\pi U$ coincide.

According to (A.1)–(A.3), the three-dimensional space of interest to us is drawn over the vectors ($\beta=1,2,3$)

$$\chi_{n\beta}=e^{ikn}(1+\varkappa_\beta u_{\rm ph}). \tag{4.20}$$

Equations (4.20) are in full agreement with Goldstone's theorem. Only two of the three functions are independent and are generated respectively by the homogeneous displacement 1 and by the phason $u_{n\rm ph}$. There are therefore only two zero-gap modes, sound and CDW, meaning that our $3\times 3$ matrix is degenerate.

The velocity $c=\varepsilon(k)/k$ of the zero-gap mode is determined, according to (1.5) by equating to zero the determinant of the matrix ($w=2Mc^2$)

$$\begin{pmatrix}1+u_1^2-F_1w & 1+u_1u_2 & 1+u_1u_3\\ 1+u_1u_2 & 1+u_2^2-F_2w & 1+u_2u_3\\ 1+u_1u_3 & 1+u_2u_3 & 1+u_3^2-F_3w\end{pmatrix},$$

where $u_\alpha=\varkappa_\alpha\langle u_{n\rm ph}^2\rangle^{1/2}$. We obtain for $w$, as expected, the equation

$$w\{w^2-w[(1+u_1^2)/F_1+(1+u_2^2)/F_2+(1+u_3^2)/F_3]+(u_1-u_2)^2/F_1F_2+(u_1-u_3)^2/F_1F_3+(u_2-u_3)^2/F_2F_3\}=0,$$

which yields only two finite velocities.

The equations obtained express in principle, with the aid of the results of Ref. 1, the velocities of the sound and of the CDW. The actual formulas, however, are in themselves not of interest, in view of the patently model-dependent character of the problem, and will not be cited here. Furthermore, the speed of sound can be directly determined from the compressibility, an expression for which is also given in Ref. 1.

## 5. STABILITY OF MULTIBAND SOLUTIONS

Formulas such as (3.12) for the second variation permit in principle, since they are patently "diagonal," investigations of the stability of multiband solutions of the variational problem (1.1)–(1.4). We verify first of all $\mu_j$ of (3.12) is posi-

tive, i.e., that the two-band (i.e., with two forbidden bands) solution investigated in Secs. 3 and 4 and in the preceeding paper[1] is stable in the case when only the smaller integral $I_2$ is retained in the elastic energy.

In the variables $\lambda = E^2$ the integral in (3.12) takes the form[1)]

$$J=\int_{\Lambda_1}^{\Lambda_2}\frac{d\lambda}{R^{1/2}(\lambda)\,(\lambda-e^2)}. \tag{5.1}$$

At $e^2<\Lambda_3$, i.e., in the central allowed band, the integrand is clearly of definite sign. Moreover, from the definition of the quasimomentum (3.3) and from the fact that it is positive and monotonic it follows that

$$-i(\lambda+C)R^{-1/2}(\lambda)>0,$$

in particular (see also Ref. 1), $\lambda + C$ reverses sign (has a root) in the interval $\Lambda_3<\lambda<\Lambda_2$. Hence

$$-i(e^2+C)R^{-1/2}(\lambda)<0$$

at $e^2<\Lambda_3$, $\Lambda_2<\lambda<\Lambda_3$, and we obtain directly

$$\mu(e^2)\sim -i(e^2+C)J>0.$$

For $e^2$ in the outer bands, the expression for $J$ can be transformed into

$$J=\int_{-\infty}\frac{d\lambda}{R^{1/2}(\lambda)\,(\lambda-e^2)},\quad \Lambda_2<e^2<\Lambda_1,$$

by simply representing $J$ in (4.1) as a contour integral and drawing an additional cut from $\Lambda_3$ to $-\infty$ (Fig. 6). The integrand is again of definite sign, and the previous arguments repeated verbating yield a positive $\mu(e^2)$.

We proceed now to the multiband solutions. As shown in the preceeding paper,[1] such states exist only when the number $l$ of the invariants $I_{2k}$ in (1.3) exceeds unity. The number $q$ of the bands does not exceed in this case $4l-2$. It will be shown below that the extremals of $\mathscr{H}$ are unstable at $q\geqslant 2l>2$.

We derive now a formula that replaces (3.12) for the $q$-band state. The same arguments as in Sec. 3 yield in lieu of (3.10) and (3.11)

$$i\delta p=(l_1E^{q+1}+\ldots+l_rE)R^{-1/2}(E)-\frac{E}{16R^{1/2}(E)}\sum_j\frac{M_q(e_j)\,(\delta e_j^2)^2}{e_j^2(E^2-e_j^2)} \tag{5.2}$$

for even $q$. Here $r=q/2+1$ and $M_q(e)$ is a known polynomial, contained in the numerator of the formula (2.5) for the quasimomentum. For odd $q$ we have

$$i\delta p=(l_1E^{q+1}+\ldots+l_r)R^{-1/2}(E)-\frac{1}{16R^{1/2}(E)}\sum_j\frac{M_q(e_j)\,(\delta e_j^2)^2}{e_j(E^2-e_j^2)}, \tag{5.3}$$

where $r=(q+1)/2+1$. We note that the polynomial $M_q(e)$ is even and does not reverse sign in the central forbidden band.

From a comparison of (3.9) with (5.2) and (5.3) it can be seen that the variations of the first $r$ invariants $\delta I_0$, $\delta I_2,\ldots,\delta I_{2r-2}$ are expressed in terms of the independent parameters $l_1,\ldots,l_r$. The variations of the remaining $\delta I_r,\ldots$ and accordingly of $\delta p$ break up into two parts: $\delta^{(1)}I_{2k}$ and $\delta^{(1)}p$, which can result from the expansion of the first term of (5.2), (5.3) in powers of $E^{-2}$, and $\delta^{(2)}I_{2k}$, and $\delta^{(2)}p$, generated by expanding the second term. (Accordingly, the energy variation of the energy takes the form 2.)

$$\delta^2\mathscr{H}=-\frac{2}{\pi}\int\delta^{(1)}pdE-P\delta^{(1)}I_0+\sum_{k=1}^{l}\varkappa_k\delta^{(1)}I_{2k}$$
$$-\frac{2}{\pi}\int\delta^{(2)}pdE+\sum_{k=r}^{l}\varkappa_k\delta^{(2)}I_{2k}.$$

The terms containing $\delta^{(1)}$ are linear algebraic relations between the $r$ quantities $l_1,\ldots,l_r$. They clearly coincide with the condition for the vanishing of the first variation of $\mathscr{H}$, considered in Ref. 1, and drop out of the second variation as in Sec. 3. Therefore

$$\delta^2\mathscr{H}=-\frac{2}{\pi}\int\delta^{(2)}pdE+\sum_{k=r}^{l}\varkappa_k\delta^{(2)}I_{2k}. \tag{5.4}$$

The appearance of the second term in (5.4) is a distinguishing feature of the multiband ($q>2$) case.

Before we proceed to investigate (5.4), we note that positiveness of $\delta^2\mathscr{H}$ certainly requires that the chemical potential be in the forbidden band. Otherwise the gap $\delta e_\mu$, which opens up at $e=\mu$, would make the typical Peierls singular negative contribution $(\delta e_\mu)^2\ln\delta e_\mu$. We have previously obtained the same result from the condition that the energy be an extremum with respect to the number of electrons.

Let now $r>l-1$. Without writing out explicitly the self-consistency equations, which are perfectly analogous to those in Ref. 1, we note that the vanishing of the coefficient of $\delta I_{2r+2}$ in $\delta\mathscr{H}$ yields

$$\int_{\Lambda_1}^{\mu^2}\frac{d\lambda}{R^{1/2}(\lambda)}=0 \tag{5.5}$$

for even $q$ and

$$\int_{\Lambda_1}^{\mu^2}\frac{d\lambda}{(\lambda R(\lambda))^{1/2}}=0 \tag{5.5'}$$

for odd $q$.

In analogy with the derivation of (3.12), we find that

$$-\frac{2}{\pi}\int[l_1E^{q+1}+\ldots+l_rE]\frac{dE}{R^{1/2}}-P\delta^2I_0+\sum_{k=1}^{l}\varkappa_k\delta^2I_{2k}=0$$

for even $q$ and a similar equality for odd $q$. For $\delta^2\mathscr{H}$ we have again Eq. (3.12), where

$$\mu_j=\frac{1}{16\pi i}\frac{M_q(e_j)}{e_j^2}\int_{\Lambda_1}^{\mu^2}\frac{d\lambda}{R^{1/2}(\lambda)\,(\lambda-e_j^2)} \tag{5.6}$$

at even $q$. At odd $q$ we have

$$\mu_j=\frac{1}{16\pi i}\frac{M_q(e_j)}{e_j}\int_{\Lambda_1}^{\mu^2}\frac{d\lambda}{(\lambda R(\lambda))^{1/2}(\lambda-e_j^2)}. \tag{5.6'}$$

The cycle $b_\mu$ (the integral from $\Lambda_1$ up to $\mu^2$) encloses a certain number of allowed bands on the $\lambda$ plane. It is necessary here to include in the allowed bands cuts $(\Lambda_{q+1},-\infty)$ for even $q$ and $(0,-\infty)$ for odd $q$ (Figs. 7a,b), and take into account the

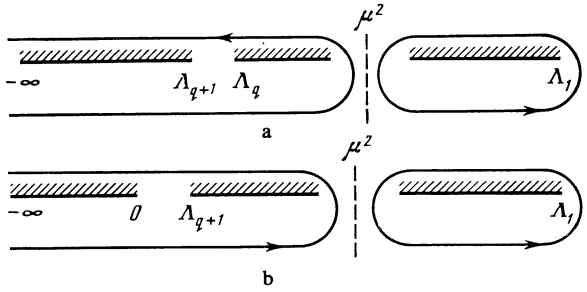


FIG. 7.

possibility of transforming from an integral from $\Lambda_1$ up to $\mu^2$ to an integral from $\mu^2$ up to $-\infty$. It will become clear later, however, that for odd $q$ the "band" $(0, -\infty)$ must not be included among the allowed bands that remain outside the contour.[3)] The reason, in final analysis, is the already mentioned fact that in this case the polynomial $M_q/e = f(e^2)$ has no roots in the interval $(0, \Lambda_{q+1})$.

Let the number of the forbidden bands that separate the allowed bands outside the contour be $u$, and let the number of the similar forbidden bands inside the contour be $v$. We do not include in $v + y$ the forbidden band that contains $\mu^2$.

Without loss of generality it can be assumed that $u \geqslant v$, for in the opposite case the integral from $\Lambda_1$ up to $\mu^2$ can be replaced in the succeeding equations, as already mentioned, by an integral from $-\infty$ to $\mu^2$.

We assume that $\mu_j$ in (5.6) and (5.6′) is of constant sign, and show that this leads to a contradiction at $q \geqslant 2l$. Since $M_q$ (or $M_q/e$ in the case of odd $q$) has simple zeros in the forbidden bands, the integrals in (5.5) and (5.6) should have $u + v$ simple zeros $\tau_s$ in the forbidden bands that are not crossed by $b_\mu$:

$$\int_{\Lambda_1}^{\mu^2} \frac{d\lambda}{R^{1/2}(\lambda)\,(\lambda-\tau_s)} = 0; \quad s=1,\ldots,u+v; \quad \tau_1<\tau_2<\ldots. \tag{5.7}$$

(The same equation holds for odd $q$ if the substitution $R(\lambda) \to \lambda R(\lambda)$ is made; the reasoning remains the same). On the other hand, we can choose $v$ points $\nu_t$; $t = 1,\ldots,v$, in the forbidden bands inside the contour and verify that the integrand in

$$\int_{\Lambda_1}^{\mu^2} \frac{d\lambda}{R^{1/2}(\lambda)} \prod_{t=1}^{v} (\lambda-\nu_t) \Big/ \prod_{s=1}^{u} (\lambda-\tau_s)$$

is of constant sign. In fact, all the differences $\lambda - \tau_s$ are negative, and the product in the numerator reverses sign by as many times as $R^{1/2}(\lambda)$. On the other hand at $v \leqslant u$ the integrand can be expanded in partial fractions:

$$\sum_{s=1}^{\bar{u}} d_s \int_{\Lambda_1}^{\mu^2} \frac{d\lambda}{R^{1/2}(\lambda)\,(\lambda-\tau_s)} + d_0 \int_{\Lambda_1}^{\mu^2} \frac{d\lambda}{R^{1/2}(\lambda)} \neq 0,$$

thus obviously contradicting (5.7) and (5.5).

Thus, states with the maximum possible number of bands, with exception of the two-band state at $l = 1$ (model $I$ in Ref. 1) are certainly unstable. By the same token, the earlier assumptions[3] that the maximum-band extremal is unconditionally preferred energywise is not confirmed.

States with a smaller number of forbidden bands must be individually studied, and this cannot be done analytically. We confine ourselves therefore to a cursory description of a case in which two Toda integrals, $\varkappa_1 I_2 + \varkappa_2 I_4$, are preserved in the elastic energy (1.3). The maximum number of unstable forbidden bands is equal to six or five.

The calculations necessary for the study of the stability of the two-band state (Fig. 1) are confined as before to the use of elliptic functions. We shall not investigate the extremum conditions,[1] but examine only the form of the second variation of (5.4). We have

$$\delta^2\mathcal{H} = -\frac{2}{\pi}\int \delta^{(2)} p\,dE + \varkappa_2 \delta^{(2)} I_4. \tag{5.8}$$

We obtain $\delta^{(2)} I_4$ by comparing the coefficients of $E^{-4}$ in (3.9) and in the second term of (5.2) [or of (3.10) and (3.11)]:

$$\delta^{(2)} I_4 = \frac{1}{16}\sum_j \frac{(e_j^2+C)\,(\delta e_j^2)^2}{e_j^2}.$$

Substituting this in (5.8) we arrive at an equation of the form (3.12) with

$$\mu_j = \frac{e_j^2+C}{16e_j^2}\left\{\varkappa_2 + \frac{2}{\pi i}\int_{E_1}^{\mu} \frac{E\,dE}{R^{1/2}(E)\,(E^2-e_j^2)}\right\}. \tag{5.9}$$

Equation (5.9) does not make $\mu_j$ positive *a priori*, since this calls for a detailed investigation of the dependence of the solutions $E_1$, $E_2$, $E_3$, $C$ of self-consistency equations on $\varkappa_2$. Nonetheless, it follows from the foregoing that $\mathcal{H}$ has no stable extremals with more than two bands. Therefore, if $\mu_j$ is no longer positive in (5.9), this can occur only if $\mathcal{H}$ is not bounded from below, as can occur in the case of negative $\varkappa_2$ with large absolute values.

## APPENDIX

We begin the calculation with the aid of (4.18) with $\langle |u_n^{\pm}|^2 \rangle$. Near $\alpha = 0$ and $P = 0$, expanding (4.17) in terms of $\alpha$ and $P$, we have

$$u_n^{\pm}(P) \approx \mp 2iP \pm 2\alpha u_{\text{ph}}$$

with $u_{n\text{ph}}$ from (4.6).

We express now $\alpha$ in terms of $P$ with the aid of (4.16):

$$iP \approx 4\omega_1'\alpha\zeta(z_{10}) - 4\alpha\eta_1' z_{10},$$

whence

$$\begin{aligned} &u_n^{\pm}(P) = \mp 2iP(1+\varkappa_1 u_{\text{ph}}), \; P \to 0, \\ &\varkappa_1 = -1/4\,[\omega_1'\zeta(z_{10}) - \eta_1' z_{10}], \\ &\langle |u_n^{\pm}|^2 \rangle = 4P^2(1+\varkappa_1^2 \langle u_{\text{ph}}^2 \rangle). \end{aligned} \tag{A.1}$$

Near $\alpha = \tau/2$ with $P \leqslant 2U$ we have

$$\begin{aligned} u_n^{\pm}(P) = &\exp[-i\pi\tau \mp 2\pi i n U + 2\pi i(2\alpha-\tau)] \\ &\times\{\exp[\mp i(P-2\pi U)]\,\theta_3(U(n-1) \\ &\pm(2\alpha-\tau)+\Phi)/\theta_3(U(n-1)+\Phi) \\ &-\exp[\pm i(P-2\pi U)]\,\theta_3(U(n+1) \\ &\pm(2\alpha-\tau)+\Phi)/\theta_3(U(n+1)+\Phi)\} \\ &\approx \exp(-i\pi\tau \mp 2\pi i n U)\,[\mp 2i(P-2\pi U) \\ &\pm(2\alpha-\tau)\,u_{\text{ph}}]. \end{aligned}$$

We have used the condition $\theta_3(v+\tau)$ is periodic.[7] The con-

nection between $2\alpha-\tau$ and $P-2\pi U$ is again obtained from (4.16) (it must be taken into account that $\tau=\omega_1/\omega_1'$):

$$i(P-2\pi U)\approx(2\alpha-\tau)\{\omega_1'[\zeta(z_{10}+\omega_1)+\zeta(z_{10}-\omega_1)]-2\eta_1'z_{10}\}.$$

We finally have

$$u_n^{\pm}(P)=\mp 2i(P-2\pi U)\exp(-i\pi\tau\mp 2\pi inU)(1+\varkappa_2 u_{\rm ph}),$$
$$P\to 2\pi U-0,$$
$$\varkappa_2=-1/2\{\omega_1'[\zeta(z_{10}+\omega_1)+\zeta(z_{10}-\omega_1)]-2\eta_1'z_{10}\},$$
$$\langle|u_n^{\pm}(P)|^2\rangle=4(P-2\pi U)^2e^{-2\pi i\tau}(1+\varkappa_2^2\langle u_{\rm ph}^2\rangle). \quad (A.2)$$

In perfect analogy, we obtain near the point $\alpha=\frac{1}{2}+\frac{1}{2}\tau$

$$u_n^{\pm}(P)=\mp 2i(P-2\pi U)\exp(-i\pi\tau\mp 2\pi inU)(1+\varkappa_3 u_{\rm ph}),$$
$$P\to 2\pi U+0,$$
$$\varkappa_3=-1/2\{\omega_1'[\zeta(z_{10}+\omega_1+\omega_1')+\zeta(z_{10}-\omega_1-\omega_1')]-2\eta_1'z_{10}\}. \quad (A.3)$$

Equations (A.2)–(A.3) with allowance for (4.17) prove (4.20).

It remains now to expand the function $\sigma$ and $\wp$ near the points $\alpha=0,\ \frac{1}{2}\ \tau,\ \frac{1}{2}+\frac{1}{2}\tau$. At $\alpha=0$ this yields

$$\frac{\mathrm{diag}_1\,\delta^2\mathcal{H}}{\mu(0)}=\frac{(4\omega_1'\alpha)^4\wp'^2(z_{10})}{4P^2(1+\varkappa_1^2\langle u_{\rm ph}^2\rangle)}$$

or, using the connection of $\alpha$ with $P$

$$\frac{\mathrm{diag}_1\,\delta^2\mathcal{H}}{\mu(0)}\approx\frac{4P^2(2\omega_1'\varkappa_1)^4\wp'^2(z_{10})}{1+\varkappa_1^2\langle u_{\rm ph}^2\rangle}. \quad (A.4)$$

Near $\alpha=\tau/2$ we have

$$\frac{\mathrm{diag}_2\,\delta^2\mathcal{H}}{\mu(\tau/2)}=\frac{\sigma^2(2\omega_1+2\omega_1'(2\alpha-\tau))}{\exp(4\eta_1'\omega_1^2/\omega_1'-2\omega_1 i\pi/\omega_1')}$$
$$\times\frac{[\wp(\omega_1+z_{10}+(2\alpha-\tau)\omega_1')-\wp(\omega_1-z_{10}+(2\alpha-\tau)\omega_1')]^2}{4(P-2\pi U)^2(1+\varkappa_2^2\langle u_{\rm ph}^2\rangle)}$$
$$\approx\exp\{2i\pi\omega_1/\omega_1'-4\eta_1'\omega_1^2/\omega_1'+4\eta_1\omega_1\}$$
$$\frac{(2\omega_1'(2\alpha-\tau))^4\wp'^2(z_{10}+\omega_1)}{4(P-2\pi U)^2(1+\varkappa_2^2\langle u_{\rm ph}^2\rangle)}.$$

Using the relation between $\alpha$ and $P$ and the known identity[7]

$$-\eta_1\omega_1'+\eta_1'\omega_1=\tfrac{1}{2}\pi i,$$

we obtain

$$\frac{\mathrm{diag}_2\,\delta^2\mathcal{H}}{\mu(\tau/2)}=(P-2\pi U)^2\frac{4(2\omega_1'\varkappa_2)^4\wp'^2(z_{10}+\omega_1)}{1+\varkappa_2^2\langle u_{\rm ph}^2\rangle}. \quad (A.5)$$

Similarly, near $\alpha=\frac{1}{2}+\frac{1}{2}\tau$ we obtain

$$\frac{\mathrm{diag}_3\,\delta^2\mathcal{H}}{\mu(\frac{1}{2}+\tau/2)}=(P-2\pi U)^2\frac{4(2\omega_1'\varkappa_3)^4\wp'^2(z_{10}+\omega_1+\omega_1')}{1+\varkappa_3^2\langle u_{\rm ph}^2\rangle}. \quad (A.6)$$

It remains for us to calculate $\mu$. In the factor preceeding the integral in (3.12) we can simply substitute respectively $E_1^2, E_2^2, E_3^2$ and $C$ from the preceeding paper.[1] To calculate the integral in (3.12) it will become necessary to use the second parametrization of Ref. 1. The variable $z_2$ is introduced with the aid of the relation

$$z_2=\frac{1}{2}\int_{\Lambda_1}^{\lambda}\frac{d\lambda}{R^{1/2}(\lambda)}.$$

The inversion is given by the Weierstrass elliptic function $\wp(z_2)$ with periods $2\omega_2$ and $2\omega_2'$, shown in Fig. 6b of Ref. 1:

$$\lambda(z_2)=\wp(z_2+\omega_2')+\Lambda_1-\wp(\omega_2').$$

The integral in (3.12) is written in the form

$$\int_0^{2\omega_2}\frac{dz_2}{\lambda(z_2)-\lambda}.$$

At the point $\alpha=0$ we must calculate

$$\int_0^{2\omega_2}\frac{dz_2}{\wp(z_2+\omega_2')-\wp(\omega_2')}.$$

We note for this purpose that the integrand itself is a linear function of $\wp(z_2)$. The concrete form is determined by the position of the zero $z_2=\omega_2'$ and of the pole $z_2=0$:

$$\frac{1}{\wp(z_2+\omega_2')-\wp(\omega_2')}=\frac{2}{\wp''(\omega_2')}(\wp(z_2)-\wp(\omega_2')).$$

For the integral we have

$$\frac{2}{\wp''(\omega_2')}(-\zeta(2\omega_2)-2\omega_2\wp(\omega_2'))$$
$$=-\frac{4}{\wp''(\omega_2')}(\eta_2+\omega_2\wp(\omega_2')).$$

Similarly, at the point $\alpha=\tau/2$ we get

$$-\frac{4}{\wp''(\omega_2+\omega_2')}(\eta_2+\omega_2\wp(\omega_2+\omega_2')),$$

and at the point $\alpha=\frac{1}{2}+\tau/2$

$$-\frac{4}{\wp''(\omega_2)}(\eta_2+\omega_2\wp(\omega_2)).$$

Combining the results, we obtain the final formula for $F_\beta$ of (4.19)

$$F_\beta=\frac{2i}{\pi}\frac{(2\omega_1'\varkappa_\beta)^4\wp'^2(z_{10}+\tilde\omega_{1\beta})}{\wp''(\tilde\omega_{2\beta})E_\beta^2}(E_\beta+C)(\eta_2+\omega_2\wp(\tilde\omega_{2\beta})), \quad (A.7)$$

where

$$\tilde\omega_{11}=0,\quad \tilde\omega_{12}=\omega_1,\quad \tilde\omega_{13}=\omega_1+\omega_1',$$
$$\tilde\omega_{21}=\omega_2,\quad \tilde\omega_{22}=\omega_2+\omega_2',\quad \tilde\omega_{23}=\omega_2'.$$

[1)] Owing to the evident symmetry of the problem we can assume that the chemical potential $\mu$ lies in the lower forbidden band, $E_2<\mu<E_3$.
[2)] For uniformity we designated the variations of the first $r$ invariants $\delta I_{2h}$ likewise by $\delta^{(1)}I_{2h}$.
[3)] On the contrary, the band $(0,-\infty)$ must be included among the bands enclosed by the contour (Fig. 7b).


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