Discrete Peierls models with exact solutions

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Exactly solvable Peierls models that contain typical continual models and the molecular limit as limiting cases are found. The interaction between the electrons and the lattice is taken into account via the exponential dependence of the electron hop-over integral on the distance between the nearest molecules. Also considered is the special case of interaction with intramolecular deformations. The thermodynamic functions, the distributions of the molecules and of the electron density, and the electron spectrum are obtained for the ground state. It is shown that at any electron density ρ the spectrum is always single-band. There are no commensurability effects at all $\rho \neq 0$, and the ground state has a zero mode.

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1. INTRODUCTION. FORMULATION OF THE MODELS.

1. It has become clear recently that the Peierls-Frŏhlich models admit of an exact solution.[1-6] Models with a linearized electron dispersion law near the Fermi level[1-3,5,6] and the Frŏhlich model with a quadratic dispersion law[4] were investigated. An independent study was made of the model of electron-phonon interaction on a discrete lattice.[7-11] This model was investigated numerically, either using variational calculations,[7,8] or by models of the dynamics equations.[9-11]

We show in this paper that there exists also a class of exactly solvable discrete models. We shall investigate two models (I, II) that include as limiting cases all the hitherto considered models of the Peierls effect, as well as the molecular limit. In Model I the interaction is taken into account only via dependence of the electron hop-over integral on the distance between the molecules. In model II, account is taken also of the interaction of the electron with the intramolecular vibrations.

The investigation reported in this paper is based on a special mathematical formalism whose description can be skipped by a reader interested only by the physical deductions. We have therefore reported the results of the research in Chaps. 2 and 3, and their derivation is expounded in Chaps. 4 and 5.

In Chap. 1 below we formulate the exactly solvable Peierls model. In Chaps. 2 and 3 we present the results of the exact solution, consider its physical consequences, and investigate various limiting cases. In Chap. 4 we present the necessary results of the spectral theory of difference operators, prove the exact solvability of the presented models, derive a complete system of self-consistency equations, and obtain expressions for the thermodynamic parameters. In Cahp. 5 we present a partial solution of the equations of Chap. 4 in terms of elliptic functions, and obtain general expressions for the electron wave functions, for the electron-density distribution, and for the equilibrium arrangement of the molecules. Individual mathematical questions are relegated to the Appendix.

2. We consider a one-dimensional chain of molecules located at the points x_n. Each group of N molecules has $N_e \leqslant 2N$ electrons. We shall assume that the electron spectrum is determined by the typical tight-binding Hamiltonian

$$H\psi_n = c_n\psi_{n+1} + c_{n-1}\psi_{n-1} + v_n\psi_n = E\psi_n, \quad c_n = c(x_{n+1} - x_n), \qquad (1.1)$$

where c_n are the integrals for the electron hopping between the nearest molecules and v_n is a local potential produced by the possible intramolecular deformation (it differs from zero only in model II). The ground state of the system is determined from the extremum condition on the energy functional of the system[1)]

$$W = \sum_{E \leqslant \mu} E + U, \qquad (1.2)$$

where the electron energy levels $E = E\{c_n, v_n\}$ are determined from (1.1), μ is the chemical potential, and $U = U\{x_n, v_n\}$ is the energy of the potential interaction between the molecules and the intramolecular strains.

Greatest interest attaches to the case of rigid lattices:

$$x_n = na + u_n, \quad |u_n| \ll a,$$

when the strains v_n and the displacements u_n of the molecules under the influence of the electrons are small enough. We can confine ourselves here to a quadratic expansion of U in u_n and v_n, and to a linear expansion of c_n in (1.1) in terms of $u_{n+1} - u_n$:

$$x_n \approx na + u_n, \quad c_n \approx c_0[1 - \alpha(u_{n+1} - u_n)],$$

$$U = \frac{1}{2}\sum_n [K(u_{n+1} - u_n)^2 + kv_n^2]. \qquad (1.3)$$

The linearized Peierls lattice model, defined by Eqs. (1.1)–(1.3) at $v_n = 0$, was formulated, e.g., in Refs. 7–11 and 13, and was investigated in Refs. 7–11.

In this paper we propose the following relations for c and U:

$$c = C_0 e^{-\alpha x}, \quad U = \sum_n \left[\frac{1}{2}kv_n^2 + \varkappa C_0^2 \exp\{-2(x_{n+1} - x_n)\}\right]. \qquad (1.4)$$

We shall show that the models defined by Eqs. (1.1) and (1.2) with the relations (1.4) can be solved exactly

in two cases, hereafter called models I and II. In model I it is assumed that there is no strain potential, $v_n \equiv 0$, an assumption corresponding to the limit $k \to \infty$. The problem with $v_n \neq 0$ can be solved only at a special value of the parameter k, namely at $k = \varkappa$. This case will be called model II.

The energy functional W should be varied at constant particle numbers N and N_e and at a constant length $L = Na$ of the system. It is more convenient to vary the functional of the adjoint thermodynamic potential

$$\tilde{W} = W + PL, \quad L = Na = x_{N+1} - x_0 = \sum_{n=0}^{N} (x_{n+1} - x_n)$$

at constant P. At equilibrium,

$$W = Nw_0(\rho, a), \quad \tilde{W} = N\mu_0(\rho, P), \quad \rho = N_e/N,$$

where $\mu_0(\rho, P)$ is the chemical potential of the molecule. It will be shown below that it is natural to express the variational functional $\tilde{W}$ in form

$$N^{-1}\tilde{W}\{c_n, v_n\} = N^{-1} \sum_{E \leqslant \mu} E + \varkappa I_2 - PI_0, \tag{1.5}$$

where

$$I_0 = I_0\{c_n, v_n\} = N^{-1} \sum_{n=0}^{N-1} \ln c_n, \quad I_2 = I_2\{c_n, v_n\} = N^{-1} \sum_{n=0}^{N-1} \left(c_n^2 + \frac{1}{2} v_n^2 \right) \tag{1.6}$$

and $E = E\{c_n, v_n\}$ are the eigenvalues of (1.1). (For model I we must put $v_n = 0$ in (1.6)). The mean distance a between the molecules in the ground state is determined from the condition

$$I_0\{c_n, v_n\} = -L/N = -a.$$

at the equilibrium values of c_n and v_n.

From the form of the functional (1.1), (1.5), (1.6) we can establish the connection between our problem and that of integrating vector differential-difference equations,[14,15] viz., Langmuir chains or the difference Korteweg-de Vries equation for model I and the Toda chain for model II. The Hamiltonian (1.1) assumes here the role of the L-operator and its eigenvalues E and the functionals (1.6) are the integrals of motion of the equations of the dynamics of the corresponding chains. It is precisely this circumstance which points to the existence of an exact solution for the models considered.

At small α the models I and II reduce to the linearized discrete model (1.1)–(1.3). Smallness of α is equivalent to large P, when

$$P/\alpha\bar{c} \approx 2\varkappa\bar{c} \gg 1, \quad \bar{c} = C_0 e^{-\alpha a}.$$

(We shall use throughout energy units C_0 and lengths α^{-1} such that $c_0 = 1$ and $\alpha = 1$.) A transition to continual models is possible in this same limit. At $\rho(2 - \rho) \ll 1$ we obtain for both models I and II a continual problem with a quadratic dispersion law.[4] At $|\rho - 1| \ll 1$ we obtain a continual problem[1-3,5,6] with a linearized dispersion law for electrons in an off-diagonal field $\Delta(x)$. In this case there is a fundamental difference between models I and II. Model I corresponds to one real field $\Delta(x) = \Delta_1(x)$. Its ground state at $\rho = 1$ has only twofold degeneracy $\Delta \to -\Delta$. Model II corresponds to a theory with a complex field $\Delta(x) = \Delta_1 + i\Delta_2$. The

FIG. 1.
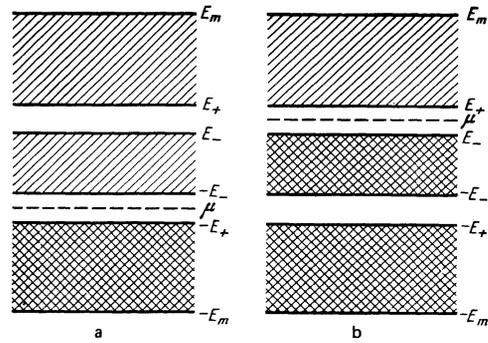
special choice $k = \varkappa$ in model II leads to the chiral invariance $\Delta \to \Delta \exp(i\chi)$, which is equivalent to the Fröhlich limit.

2. RESULTS OF SOLUTION OF MODEL I

The investigation expounded in Chap. 4 leads to the following general conclusions for the model I. The spectrum of the electron states for all $\rho \neq 0, 1, 2$ consists of three allowed bands[2]

$$-E_m \leqslant E \leqslant -E_+, \quad -E_- \leqslant E \leqslant E_-, \quad E_+ \leqslant E \leqslant E_m,$$

as shown in Fig. 1. The electron chemical potential μ is always located in one of the forbidden bands:

$$-E_+ < \mu < -E_-, \quad 0 < \rho < 1,$$
$$E_- < \mu < E_+, \quad 1 < \rho < 2.$$

At all $\rho \neq 0, 1, 2$ the ground state is continuously degenerate in some parameter t, i.e., besides the homogeneous shift there is also one zero mode. As $\rho \to 1$ this mode corresponds to an arbitrary shift of the soliton superlattice, and at $|\rho - 1| \lesssim 1$ it corresponds to the Fröhlich phase of the complex order parameter.

The entire analysis was carried out for an integer number of electrons N_e on the lattice, i.e., at rational $\rho = N_e/N$. In the thermodynamic limit $N \to \infty$ and $N_e \to \infty$, where ρ can be regarded as an arbitrary albeit generally speaking rational number, all the physical quantities were found to be continuous analytic functions of ρ everywhere except at the points $\rho = 0, 1, 2$. Thus, in this model there is no difference between rational and irrational values of ρ. Consequently all the commensurability effects except the special case of the doubling of the period at $\rho = 1$ are absent.

The foregoing conclusions show that the properties of the considered discrete model agree qualitatively with the properties of the continual models. Moreover, in analogy with the continual models, all the physical quantities are expressed in terms of elliptic functions. The relation between the physical quantities of model I are expressed in Chap. 5 in terms of the Weierstrass elliptic functions $\mathscr{P}$, ζ, and σ. For numerical calculations it is more convenient to use the standard tabulated Jacobi functions and Legendre integrals. We shall give here the results of Chap. 5 expressed in terms of Jacobi functions, using verbatim the notation of the Bateman-Erdelyi tables.[16]

The Weierstrass functions $\mathscr{P}(z)$ etc. depend on two periods ω and ω'. The Jacobi functions $\theta_i(v)$ depend on one parameter τ:

$$\tau = -\omega/\omega', \quad \mathrm{Im}(\omega'/\omega) > 0; \quad \theta_i(v) = \theta_i(v, \tau), \quad \theta_i(0) = \theta_i.$$

The Jacobi functions $\mathrm{sn}\,u$, $\mathrm{cn}\,u$, ... depend on an elliptic modulus k such that

$$K'/K = -i\tau, \quad K = K(k), \quad K' = K(k'), \quad k^2 + k'^2 = 1,$$

where $K(k)$ is a complete elliptic integral of the first kind. The set of variables z, v, u is related here by

$$v = z/2\omega' = u/2K.$$

Chapter 5 gives all the relations in the parametrizations ω_1, ω_1' and ω_2, ω_2'. We shall use the Jacobi functions only for the first parametrization, i.e, $\tau = \omega_1/\omega_1'$ etc. We shall use the symbol r for the elliptic modulus k_2' in the second parametrizations, and for the elliptic integrals in the second parametrization we shall indicate explicitly the value of the modulus $K_2' \equiv K(r)$, etc.

Equations (5.18) and (5.20) yield expressions for the band boundaries

$$E_m^2 = \frac{K}{\omega_1'}\frac{\mathrm{dn}\,u}{\mathrm{sn}\,u\,\mathrm{cn}\,u}, \quad u = K|\rho - 1|, \tag{2.1}$$

$$E_+/E_m = \mathrm{sn}\,u; \quad E_-/E_+ = k'/\mathrm{dn}\,u.$$

From (5.18) we obtain the connections between the two parametrizations

$$r^2 = \frac{E_m^2 - E_+^2}{E_m^2 - E_-^2} = \mathrm{dn}^2 u, \quad \frac{K^2(r)}{|\omega_2|^2} = \frac{K}{\omega_1'}\frac{\mathrm{cn}\,u}{\mathrm{sn}\,u\,\mathrm{dn}\,u}. \tag{2.2}$$

The period ω_2 is known from (5.20): $\omega_2 = \pi\varkappa/2$, and the ratio K/ω_1' can be explicitly expressed in terms of the mean distance a between the ions by using (5.21):

$$\frac{K}{\omega_1'} = 4e^{-2a}\,\mathrm{sn}\,u\,\mathrm{cn}\,u\,\frac{\theta_3(v)\theta_4^3(v)}{\theta_3\theta_4^3},$$

where, in accord with the definitions

$$v = \tfrac{1}{2}|\rho - 1|. \tag{2.3}$$

Substituting this in (2.2) we obtain an equation for the elliptic modulus k in terms of the parameters $\varkappa$, a, and ρ of the problem:

$$\frac{K(r)}{\mathrm{cn}\,u}\frac{\theta_4^2}{\theta_4^2(v)} = \pi\varkappa\bar{c}, \quad r = \mathrm{dn}\,u, \tag{2.4}$$

where $\bar{c}$ is the average hop-over integral

$$\bar{c} = e^{-a}, \quad \pi\varkappa\bar{c} = 1/\lambda.$$

For E_m we have then the formula

$$E_m = 2\bar{c}\theta_3(v)\theta_4(v)/\theta_3\theta_4, \tag{2.5}$$

and E_+ and E_- are obtained from (2.1) knowing k and E_m.

The thermodynamic relations are obtained by substituting the value of $k = k(a, \rho)$ determined from (2.4) in the formulas for the pressure P and the ground-state energy w_0. From (5.20b) we obtain

$$P = \frac{2}{\pi^2\varkappa}K^2(r)\left[1 + \frac{\mathrm{sn}^2 u\,\mathrm{dn}^2 u}{\mathrm{cn}^2 u} - 2\frac{E(r)}{K(r)}\right]. \tag{2.6}$$

From (5.22) we get

$$w_0 = \frac{K^2(r)}{\pi^2\varkappa}\left[1 + \frac{\mathrm{sn}^2 u\,\mathrm{dn}^2 u}{\mathrm{cn}^2 u} - 4\frac{E(r)}{K(r)} - \frac{1}{K}\mathrm{sn}(u, k)\frac{\theta_3'(|\rho - 1|/2)}{\theta_3(|\rho - 1|/2)}\right]. \tag{2.7}$$

the molecule displacements u_n can be obtained from (5.24)

$$u_n = x_n - x_0 - na = \frac{1}{2}\begin{cases} \ln\dfrac{\theta_4[|\rho - 1|(n - n_0 - 1)/2]}{\theta_4[|\rho - 1|(n - n_0 + 1)/2]}, & n = 2m, \quad (2.8) \\[2ex] \ln\dfrac{\theta_4[|\rho - 1|(n - n_0 - 1)/2 + 1/2]}{\theta_4[|\rho - 1|(n - n_0 + 1)/2 + 1/2]}, & n = 2m + 1. \end{cases}$$

We emphasize that n_0 is an arbitrary number, not necessarily an integer. The continuous ground-state degeneracy parameter n_0 constitutes the zero mode, mentioned at the beginning of this chapter, of the ground state of the system.

The distribution of the electron density ρ_n,

$$\rho_n = 2\sum_{E < \mu}\psi_n^*(E)\psi_n(E),$$

is given by Eq. (5.25). Comparing (5.24) and (5.25) we get

$$\rho_n - \rho = \frac{2}{\pi|\rho - 1|}\frac{K'}{K}\frac{\partial}{\partial n_0}u(n - n_0), \quad u(n - n_0) = u_n, \tag{2.9}$$

or

$$\rho_n - \rho = \frac{1}{\pi|\rho - 1|}\frac{K'}{K}\frac{\partial}{\partial n_0}\ln\frac{\theta_\alpha[|\rho - 1|(n - n_0 - 1)/2]}{\theta_\alpha[|\rho - 1|(n - n_0 + 1)/2]}, \tag{2.10}$$

where $\alpha = 3$ at $n = 2m + 1$ and $\alpha = 4$ at $n = 2m$.

As seen from (2.4), the ground state of the system is determined by the parameters ρ and $\varkappa\bar{c}$. We consider now the most important limit corresponding to the linearized model (1.1), (1.3). As indicated in Chap. 1, this limit corresponds to small α or, in dimensionless variables, to the inequalities

$$P \gg \bar{c}, \quad \varkappa\bar{c} \gg 1.$$

From Eq. (2.4) at $\varkappa\bar{c} \gg 1$ we find that $r \to 1$ for all ρ. It is convenient to use in place of (2.5) the interpolation formula

$$kK = \frac{2}{\sin(\pi|\rho - 1|/2)}\exp\left\{-\frac{1}{\lambda}\cos\frac{\pi|\rho - 1|}{2}\right\}, \quad \lambda \ll \cos\frac{\pi|\rho - 1|}{2}, \tag{2.11}$$

which is valid both at $|\rho - 1| \gg e^{-1/\lambda}$ and at $|\rho - 1| \ll e^{-1/\lambda}$. The quantity $\lambda/\cos(\pi|\rho - 1|/2)$ in (2.11) corresponds to the usual definition of the dimensionless electron-phonon interaction constant. Linearization of our model corresponds thus also to the weak-binding model. This is due to the presence of only one constant $\varkappa$ in the functional (1.5).

Substituting (2.11) in (2.1) we obtain at $|\rho - 1| \gg e^{-1/\lambda}$

$$E_+/E_m \approx E_-/E_m \approx \sin(\pi|\rho - 1|/2), \quad E_m \approx 2\bar{c}, \tag{2.12a}$$

$$E_+^2 - E_-^2 = 64\bar{c}^2\cos^2\frac{\pi|\rho - 1|}{2}\exp\left\{-\frac{2}{\lambda}\cos\frac{\pi|\rho - 1|}{2}\right\}. \tag{2.12b}$$

Expressions (2.12) go over at $|\rho - 1| \ll 1$ into the relations of the continual model[3,6] with a linearized dispersion law. The additional dependences on ρ in (2.12) are reflections of the curvature of the electron spectrum and of the finite width of the electron band.

At $|\rho - 1| \ll e^{-1/\lambda}$ we have from (2.1) and (2.5)

$$E_m = 2\bar{c}, \quad E_+ = 8\bar{c}e^{-1/\lambda}; \quad E_-/E_+ = 4\exp\{-4e^{-1/\lambda}/|\rho - 1|\}.$$

This region corresponds to the limit of a widely spaced soliton lattice. From (2.8) we obtain the lattice deformation in the absence of a soliton:

$$u_{2n} = \frac{1}{2} \ln \frac{\text{ch}\{\delta^{-1}[2(n-n_0)-1]\}}{\text{ch}\{\delta^{-1}[2(n-n_0)+1]\}} \approx \frac{1}{\delta}\,\text{th}\,\frac{2(n-n_0)}{\delta},$$
(2.13)

$$4\delta = e^{1/\lambda}, \quad u_{2n} \to \pm\delta^{-1}, \quad n \to \pm\infty; \quad u_{2n+1} = \text{const},$$

and the electron-density distribution

$$\rho_{2n} - \rho = \frac{1}{2}\left[\text{th}\,\frac{2(n-n_0)-1}{\delta} - \text{th}\,\frac{2(n-n_0)+1}{\delta}\right] \approx -1/\delta\,\text{ch}^2\,\frac{2(n-n_0)}{\delta}, \quad \rho_{2n+1} = \rho.$$
(2.14)

Equations (2.13) and (2.14) correspond to the single-soliton solutions of the Toda-chain equations.[14,15]

3. RESULTS OF SOLUTION OF MODEL II

The qualitative conclusions of the investigation of model II agree in general with the results given at the beginning of Chap. 2 for model I. What distinguishes model II is that it has no singularities of the physical quantities at $\rho = 1$. The electronic-state spectrum contains now only two allowed bands, (E_1, E_2) and (E_3, E_4). The chemical potential μ lies in the forbidden band (E_2, E_3)

$$E_1 \leqslant E \leqslant E_2, \quad E_3 \leqslant E \leqslant E_4, \quad E_2 < \mu < E_3.$$

In contrast to model I, the gap in the state density lies only on the Fermi surface, i.e., the spectrum has no electron-hole symmetry (see Fig. 2).

The physical quantities in model II are determined with the aid of the elliptic parametrization described in Chap. 5. Just as for model I, it is convenient to express the results in terms of Jacobi elliptic functions and theta functions. We introduce again the parameters τ and k:

$$\tau = -\omega/\omega' = iK'/K, \quad K = K(k),$$
(3.1)

where ω and ω' are the half-periods of the elliptic functions shown in Fig. 5 below. From (5.10), taking (5.5) and (5.6) into account, we obtain an equation for the parameter τ:

$$|\tau| \frac{\theta_2 \theta_3 \theta_4}{\theta_1(\rho/2)} = \varkappa\bar{c}.$$
(3.2)

The positions of the band boundaries are determined from (5.2a). Transforming it in analogy with the formulas for the model I, we obtain for the widths D of the total band, ε_F of the filled band, and E_g of the forbidden band the expressions

$$D = E_4 - E_1 = 4\bar{c}\,\frac{\theta_3^2(\rho/4)\,\theta_4^2(\rho/4)}{\theta_3^2 \theta_4^2},$$
(3.3)

$$\frac{\varepsilon_F}{D} = \frac{E_3 - E_1}{E_4 - E_1} = \text{sn}^2 u,$$
(3.4)

$$\frac{E_g}{\varepsilon_F} = \frac{E_3 - E_2}{E_3 - E_1} = k^2 \frac{\text{cn}^2 u}{\text{dn}^2 u}, \quad u = \frac{\rho}{2}K.$$
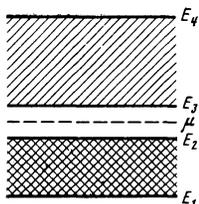(3.5)

FIG. 2.

In the weak-coupling limit $\varkappa\bar{c}\sin(\pi\rho/2) \gg 1$ it follows from (3.2) that

$$k = 4\exp\left(-\frac{1}{2\lambda}\sin\frac{\pi\rho}{2}\right); \quad \lambda = \frac{1}{\pi\varkappa\bar{c}}, \quad k \ll 1.$$
(3.6)

Equations (3.3)–(3.5) take the form

$$D \approx 4\bar{c}, \quad \frac{\varepsilon_F}{D} \approx \sin^2\frac{\pi\rho}{2},$$

$$\frac{E_g}{D} \approx 4\sin^2\frac{\pi\rho}{2}\exp\left(-\frac{1}{\lambda}\sin\frac{\pi\rho}{2}\right).$$

The equilibrium coordinates x_n of the molecules are defined in (5.13a). From this equation we obtain by simple transformation

$$u_n = x_n - x_0 - na = -\frac{1}{2}\ln\frac{\theta_4(\frac{1}{2}\rho(n-\nu-\frac{1}{2}))}{\theta_4(\frac{1}{2}\rho(n-\nu+\frac{1}{2}))}.$$
(3.7)

We note that ν is an arbitrary number, not necessarily an integer, a reflection of the continuous degeneracy of the ground state.

Comparing (5.13a) and (5.13b), we obtain for the intramolecular strains v_n

$$v_n = \frac{4|\tau|}{\pi\varkappa\rho}\frac{\partial u_n}{\partial n}.$$
(3.8)

Equation (3.8) determines also the distribution of the electron density

$$\rho_n = 2\sum_{E<\mu}\psi_n^*\psi_n = \varkappa v_n.$$

The relation $\rho_n = \varkappa v_n$ is obtained by explicit variation of the functional (1.5) with respect to v_n. In the weak-coupling limit we obtain

$$u_n = x_n - x_0 - na \approx 2\sin\left(\frac{\pi\rho}{2}\right)\exp\left[-\pi\varkappa\bar{c}\sin\frac{\pi\rho}{2}\right]\sin[\pi\rho(n-\nu)],$$
(3.9)

$$\rho_n - \rho = \varkappa v_n - \rho \approx 2(E_g/D)\cos[\pi\rho(n-\nu)].$$
(3.10)

Equations (3.9) and (3.10) yield the amplitude of the lattice deformations and the charge-density waves in the Peierls state.

4. DETERMINATION OF THE GROUND STATES FOR MODELS I AND II, AND ELEMENTS OF THE SPECTRAL THEORY OF THE SCHRÖDINGER DIFFERENCE OPERATOR

1. The solutions of the problems formulated in Chap. 1 are based on an investigation of the spectral differences of the Schrödinger difference operator H. The operators (1.1) with the periodic coefficients $c_n = c_{n+N}$, $v_n = v_{n+N}$ were actively investigated in the last few years[14,17–19] in connection with the problem of integrating the Toda-chain equations. Later in this chapter, as well as in the Appendices, we shall derive the needed results of this theory, mainly on the basis of papers by one of us.[18,19] Included among them will be certain important formulas, not found in the mathematical literature, for the eigenfunctions of the operator H, for the state density, and for the variational derivatives with respect to c_n and v_n.

The exposition in the present paper is sufficiently self-contained, so that reference to the mathematical literature is not obligatory. It will be easier, however, to read the chapters that follow by first becoming acquainted with Chap. II of Ref. 15.

The modern approach to spectral problems for periodic operators is based on an investigation of the analytic properties of the solutions of Eq. (1.1) for all values of the parameter E, including complex ones.

For any E, the space of the solutions of (1.1) is two-dimensional. By specifying arbitrary values of ψ_0 and ψ_1, all the remaining values of ψ_n can be obtained from (1.1) by recurrence. The standard basis $\varphi_n(E)$ and $\theta_n(E)$ is specified by the normalization conditions

$$\varphi_0=1, \quad \varphi_1=0; \quad \theta_0=0, \quad \theta_1=1.$$

It follows from the recurrence procedure for calculating φ_n and θ_n that $\varphi_n(E)$ and $\theta_n(E)$ are polynomials in E.

Any solution y_n of Eq. (1.1) is of the form

$$y_n=a\varphi_n+b\theta_n, \quad a=y_0, \quad b=y_1.$$

We shall consider the operators (1.1) with periodic coefficients

$$c_{n+N}=c_n, \quad v_{n+N}=v_n,$$

with an aim at going eventually to the limit as $N\to\infty$. Since H is periodic, a displacement by the period N transforms the solutions of Eq. (1.1) into solutions of the very same equation

$$y_{n+N}=a'\varphi_n+b'\theta_n.$$

The new coordinates a' and b' of the vector y_{n+N} in the basis φ_n, θ_n is expressed in terms of the old ones with the aid of the matrix T:

$$\begin{pmatrix} a' \\ b' \end{pmatrix} =T\begin{pmatrix} a \\ b \end{pmatrix}, \quad T=\begin{pmatrix} \varphi_N & \theta_N \\ \varphi_{N+1} & \theta_{N+1} \end{pmatrix}.$$

For any two solutions of (1.1), particularly for θ_n and θ_n, the expression (the analog of the Wronskians in differential equations)

$$c_n(\varphi_n\theta_{n+1}-\varphi_{n+1}\theta_n)$$

does not depend on n. Since $c_0=c_N$, we have

$$\det T=\varphi_N\theta_{N+1}-\varphi_{N+1}\theta_N=\varphi_0\theta_1-\varphi_1\theta_0=1.$$

The eigenvalues Λ of the matrix T are determined from the equation

$$\Lambda^2-2Q(E)\Lambda+1=0, \quad Q(E)=\tfrac{1}{2}[\varphi_N(E)+\theta_{N+1}(E)]. \quad (4.1)$$

The polynomial $Q(E)$ is of degree N, and its leading terms are of the form

$$Q(E)=(2c_0c_1\ldots c_{N-1})^{-1}\left[E^N-E^{N-1}\sum_{n=0}^{N-1}v_n \right.$$

$$\left. +E^{N-2}\left(\sum_{0\leqslant i<j} v_iv_j-\sum_{n=0}^{N-1}c_n^2\right)+O(E^{N-3}) \right]. \quad (4.2)$$

For the periodic problem $\psi_{n+N}=\psi_n$, i.e., for $\Lambda=1$, there are N energy levels $E^{(+)}$ determined from the equation $Q(E^{(+)})=1$. There are also N real eigenvalues $E^{(-)}$ of the antiperiodic problem $\psi_{n+N}-\psi_n$, i.e., $\Lambda=-1$. They are determined from the equation $Q(E^{(-)})=-1$.

Since $E^{(+)}$ and $E^{(-)}$ are real and since the degree of the polynomial Q is N, it follows that the inequality $|Q(E)|\gg 1$ holds at the extrema $dQ/dE=0$. A typical plot of $Q(E)$ is shown in Fig. 3.
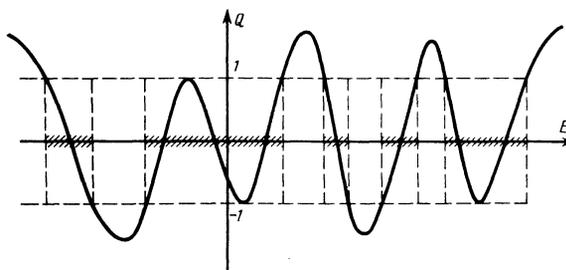

FIG. 3.

The allowed bands are segments of the E axis at which $|Q(E)|\leqslant 1$ (singled out in Fig. 3). On these segments we have as a result of (4.1)

$$|\Lambda(E)|=1; \quad \Lambda(E)=e^{ipN}, \quad p=p(E),$$

where $\pm p(E)$ are the quasimomenta corresponding to the eigenstates of the operator (1.1) with energy E. For arbitrary values of c_n and v_n, all the points $E^{(+)}$ and $E^{(-)}$ are generally speaking different and there are $N+1$ allowed bands. If the plot of the polynomial $Q(E)$ is tangent to the lines $Q=\pm 1$, so that some closest values of $E^{(+)}$ and $E^{(-)}$ merge, the neighboring allowed bands also merge and the number q of different bands will be less than $N+1$.

Let $E_1<E_2<\ldots<E_{2q+2}$ be simple roots of the equation $Q^2(E)=1$, $q<N$. The segments (E_{2j-1}, E_{2j}), $1\leqslant j \leqslant q+1$ are then allowed bands of the operator H, which will be called a q-band operator.

We shall be interested below in operators H with a finite number of bands in the limit when the chain length is infinite

$$N\to\infty, \quad q=\text{const}.$$

In this limit the levels E fill densely the allowed bands and it is possible to change from summation over the states to integrals with respect to E:

$$\sum_E \to \frac{N}{2\pi}\int dp=\frac{N}{\pi}\int \frac{dp}{dE}dE. \quad (4.3)$$

(Expression (4.3) take into account the double degeneracy of the energy with respect to the momentum, $p\to -p$.) From (4.1) and from the definition of p it follows that

$$idp=\frac{1}{N}\frac{d\Lambda}{\Lambda}=\frac{N^{-1}dQ}{\pm(Q^2-1)^{1/2}}=\frac{F(E)}{\pm R^{1/2}(E)};$$

$$R(E)=\prod_{k=1}^{2q+2}(E-E_k), \quad (4.4)$$

where $F(E)$ is a polynomial of degree q. The last equation in (4.4) follows from the fact that at the double roots of the polynomial Q^2-1, i.e., when the bands merge, the zeros of the numerator and denominator in (4.4) cancel out. The sign in front of the square root in (4.4) should be chosen such that $dp>0$.

Since the operator H has no eigenvalues inside the forbidden bands, we have

$$\int_{E_{2j}}^{E_{2j+1}} \frac{dp}{dE} dE = 0, \quad j = 1, \dots, q.\tag{4.5}$$

This system enables us to find, in quadratures, the coefficients of the polynomial $F(E)$. It must be added that the integrals of dp over the allowed bands are of the form

$$\frac{1}{\pi} \int_{E_{2j-1}}^{E_{2j}} dp = \frac{m_j}{N}, \quad \sum_j m_j = N,\tag{4.6}$$

where m_j are integers equal to the number of merging bands.

It follows from (4.4) that the differential dp is single-valued on the Riemann surface Γ of the function $R^{1/2}(E)$. We shall represent such a surface as two glued-together E planes with cuts along the allowed bands, such that the upper edge of the cut on one of the sheets is glued to the lower edge of the cut on the second sheet. The upper sheet of Γ will be designated as the sheet on which we choose, in the vicinity of infinity, $E \to \infty$, the following $R^{1/2}(E)$ branch:

$$R^{1/2}(E) = E^{q+1} + O(E^q).$$

It follows from (4.4) that $dp > 0$ on the upper edges of the cuts on the lower sheet. To obviate the need for stipulating each time the sign of the square root in (4.4) and in the equations that follow, we integrate on the Γ surface along cycles a_j that close the allowed bands (E_{2i-1}, E_{2i}), $i = 1, \dots, q+1$, see Fig. 4 here and Figs. 6–9 of Ref. 15.

For the variation of the quasimomentum with respect to c_n and v_n we have the formula

$$i\delta p = R^{-1/2}(E) \sum_{i=0}^{q+1} l_i E^{q+1-i},\tag{4.7}$$

which is derived in Appendix 1. The coefficients l_i in (4.7) contain the differentials δc_n and δv_n. To find these coefficients we use the following device.

Consider the expansion of $p(E)$ in the vicinity of infinity on the upper sheet

$$ip = N^{-1} \ln \Lambda = \ln E - I_0 - I_1 E^{-1} - I_2 E^{-2} - \dots - I_k E^{-k} - \dots.\tag{4.8}$$

From the definition of Λ and from (4.2) it follows that

$$I_0 = N^{-1} \sum_{n=0}^{N-1} \ln c_n, \quad I_1 = N^{-1} \sum_{n=0}^{N-1} v_n,$$

$$I_2 = N^{-1} \sum_{n=0}^{N-1} \left(\frac{1}{2} v_n^2 + c_n^2 \right);\tag{4.8a}$$

I_k is a polynomial of degree k in c_n and v_n. We note that the notation introduced here for I_0 and I_2 matches that of Eqs. (1.6). Expanding (4.7) in powers of E^{-1}, we obtain
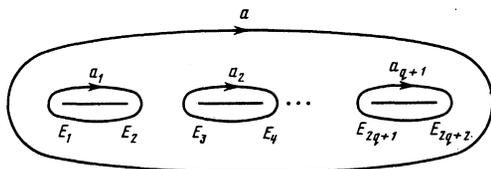

$$a$$

FIG. 4.

$$\left[\sum_{i=0}^{q+1} l_i E^{-i} \right] \left[1 + \sum_{m=1}^{\infty} G_m E^{-m} \right] = -\sum_{k=0}^{\infty} \delta I_k E^{-k},$$

where G_m are symmetric functions of E_j raised to the degree m, and are the coefficients of the expansion of the function $E^{q+1} R^{-1/2}(E)$ in powers of E^{-1}. From this equation we get

$$l_0 = -\delta I_0, \quad l_1 = -\delta I_1 + \tfrac{1}{2} s_1 \delta I_0,$$
$$l_2 = -\delta I_2 + \tfrac{1}{2} s_1 \delta I_1 - (\tfrac{1}{8} s_1^2 - \tfrac{1}{2} s_2) \delta I_0;$$
$$s_1 = \sum_{j=1}^{2q+2} E_j, \quad s_2 = \sum_{k>j} E_k E_j.$$

The general expression for l_i is

$$l_i = \sum_{j=0}^{i} \alpha_{ij} \delta I_j, \quad \alpha_{ii} = -1.\tag{4.9}$$

It follows from (4.9) that not more than $q+1$ of the differentials δI_k are linearly independent. In fact, δI_k are linear combinations of l_i. Since the latter are linear functions of δI_i, $i \leq q+1$, it follows that δI_k are also linear combinations of δI_i. An important statement of the theory of "finite-band operators" H (see Appendix 1) is that δI_i, $i \leq q+1$ are linearly independent for q-band operators.

2. We now apply the results above to the problem of the ground states of the models I and II. We begin with model II, which is technically somewhat simpler. Variation of (1.5) yields in the limit as $N \to \infty$

$$0 = N^{-1} \delta W = \frac{2}{\pi} \delta \int_{E_1}^{\mu} E dp + \varkappa \delta I_2 - P \delta I_0.$$

We recognize that the variation is over a fixed number of electron (constant ρ):

$$\frac{2}{\pi} \int_{E_1}^{\mu} dp = \rho.$$

In addition, we confine ourselves for the time being to variation at fixed band boundaries $E_1, \dots, E_{2q+2}$. If μ is in allowed bands, the condition that p be constant calls for variation of μ. We have

$$\delta \int_{E_1}^{\mu} dp = \left(\frac{dp}{dE} \right)_\mu \delta\mu + \int_{E_1}^{\mu} d(\delta p) = \left(\frac{dp}{dE} \right)_\mu \delta\mu + (\delta p)_\mu = 0.$$

We use this relation in the calculation of the variation of the electric energy:

$$\delta \int_{E_1}^{\mu} E dp = \mu \left(\frac{dp}{dE} \right)_\mu \delta\mu + \int_{E_1}^{\mu} E d\delta p = \mu \left(\frac{dp}{dE} \right)_\mu \delta\mu + \mu(\delta p)_\mu - \int_{E_1}^{\mu} \delta p dE.$$

The first two terms cancel out here, and the variation of the total energy $\bar{W}$ takes the form

$$-\frac{2}{\pi} \int_{E_1}^{\mu} \delta p dE + \varkappa \delta I_2 - P \delta I_0 = 0.$$

Obviously, the equation does not change if μ is in a forbidden band. In this case it is necessary to replace μ in the upper limit by the boundary of the upper allowed band. In Appendix 3 the variation was carried out also with respect to the band boundaries. It shows that μ is in fact always located in a forbidden band.

Using now δp from (4.7) and (4.9), we express the variation $\delta \bar{W}$ in the form[3]

$$x\delta I_2 - P\delta I_0 + \frac{2}{\pi} i \sum_{k=0}^{q+1} \delta I_k \sum_{j=0}^{q-k+1} \alpha_{kj} \int_{E<\mu} \frac{E^j dE}{R^{\prime\prime}(E)}. \qquad (4.10)$$

By the same token the problem of finding the extremals, which is generally speaking functional, reduces to solution of a finite number of algebraic relations. This is due to two factors: the finite-band character of the spectrum of the operator H for any extremal, and the special choice of the deformation energy in the form of a linear combination of the integrals I_0 and I_2. The finite-band character of the spectrum of H under the condition that the deformation energy is a linear combination of a finite number of integrals I_k is proved in Appendix 2. In particular, for our choice of the deformation energy there is only one forbidden band.

The condition (4.10) yields $q+2$ algebraic relations:

$$\int_{E<\mu} E^k R^{-1/2}(E)\,dE = \int_{E>\mu} E^k R^{-1/2}(E)\,dE, \quad 0 \leqslant k \leqslant q-2, \qquad (4.11)$$

$$x = \frac{2}{\pi} i \int_{E<\mu} E^{q-1} R^{-1/2}(E)\,dE, \qquad (4.12a)$$

$$0 = \int_{E<\mu} \left[E^q - \frac{s_1}{2} E^{q-1} \right] R^{-1/2}(E)\,dE, \qquad (4.12b)$$

$$P = -\frac{2}{\pi} i \int_{E<\mu} \left[E^{q+1} - \frac{s_1}{2} E^q + E^{q-1} \left(\frac{s_2}{2} - \frac{s_1^2}{8} \right) \right] R^{-1/2}(E)\,dE. \qquad (4.12c)$$

(The equality of the integrals with respect to $E > \mu$ and $E < \mu$ in (4.11) can be easily proved by considering the integral over the cycle a, shown in Fig. 4.) We shall show that Eqs. (4.11) have no solutions at $q > 2$. Bearing in mind the two forms of Eq. (4.11), we can assume that the region $E < \mu$ contains not less than $[q/2]$ forbidden bands ($[q/2] = q/2$ if q is even, and $[q/2] = (q-1)/2$ if q is odd).

Let $\mu_s < \mu$ be arbitrary points located one in each forbidden band to the left of μ. The auxiliary function

$$-iR^{-1/2}(E) \prod_s^{[q/2]} (E - \mu_s)$$

has then the same sign in all the allowed bands to the left of μ. (It is easy to verify that $iR^{1/2}(E)$ reverses sign on going from band to band. According to the choice of μ_s, the numerator also changes sign in this transition.)

Thus,

$$-i \int_{E<\mu} \prod_s^{[q/2]} (E - \mu_s) R^{-1/2}(E)\,dE \neq 0,$$

which contradicts (4.11) if the degree $[q/2]$ of the polynomial

$$\prod_s^{[q/2]} (E - \mu_s),$$

is less than or equal to $q-2$. Consequently $q \geqslant 2$. We have proved that the spectrum of the Hamiltonian H has not more than two forbidden bands.

At $q = 2$ only one of the equations in (4.11) is left:

$$\int_{E<\mu} R^{-1/2}(E)\,dE = \int_{E>\mu} R^{-1/2}(E)\,dE = 0.$$

It can be satisfied only if μ lies strictly inside the central forbidden band: $E_3 < \mu < E_4$. Otherwise one of the integrands is of fixed sign. It will be shown in Appendix 3, however, that the chemical potential μ is always in a forbidden band. We are left therefore with the only possibility $q = 1$. We have thus shown that the operator H, which corresponds to the extremals of $\tilde{W}$, always have one and only one forbidden band (E_2, E_3) situated between two allowed bands (E_1, E_2) and (E_3, E_4), and the lower band (E_1, E_2) is completely filled.

The three self-consistency equations for the determination of the four parameters E_i take the form (4.12) at $q = 1$. The fourth equation is the definition of the electron density ρ. It follows from (4.4) that at $q = 1$ the expression for the state density takes the form

$$-\frac{2}{\pi} \frac{dp}{dE} = \frac{2}{\pi} [-R(E)]^{-1/2} [E+Q], \quad R(E) = \prod_{i=1}^4 (E - E_i), \qquad (4.13)$$

where Q is determined from the condition (4.5):

$$\int_{E_1}^{E_2} dp = 0, \quad Q = -\int_{E_1}^{E_2} E R^{-1/2}(E)\,dE \bigg/ \int_{E_1}^{E_2} R^{-1/2}(E)\,dE. \qquad (4.14)$$

With the aid of (4.13) we obtain

$$\rho = -\frac{2}{\pi} \int_{E_1}^{E_2} \frac{dp}{dE}\,dE = -\frac{2}{\pi} \int_{E_1}^{E_2} (E+Q)[-R(E)]^{-1/2}\,dE. \qquad (4.15)$$

Equations (4.12) at $q = 1$ together with (4.14) and (4.15) determine uniquely the parameters E_i.

To express the energy Nw_0 and the length Na of the system in terms of E_i we must calculate the functionals I_0 and I_2 defined in (4.8a) or (1.6). To this end we expand (4.13) and (4.15) in powers of E^{-1} and compare the expansion coefficients with (4.8). We obtain

$$I_1 = \tfrac{1}{2} s_1 + Q, \qquad (4.16)$$

$$I_2 = \tfrac{1}{16}(3s_1^2 - 4s_2 + 4Qs_1), \qquad (4.17)$$

$$I_0 = \lim_{E \to \infty} \left[\ln E - \int_{E_1}^E (E+Q) R^{-1/2}(E)\,dE \right]. \qquad (4.18)$$

The integral in (4.18) is over the upper sheet of the surface Γ.

With the aid of (4.13) and (4.17), using (4.12a) and (4.12c), we obtain from (1.5) for the system ground-state energy Nw_0

$$w_0 = \frac{2}{\pi} \int_{E_1}^{E_2} E \frac{dp}{dE}\,dE + x I_2 = P + \frac{1}{4} s_1 \rho + \frac{1}{4} x \left(s_2 - \frac{1}{4} s_1^2 \right). \qquad (4.19)$$

3. To conclude this chapter, we summarize briefly the results for model I. At $v_n = 0$, each solution $\psi_n(E)$ of (1.1) corresponds to a solution

$$\psi_n(-E) = (-1)^n \psi_n(E).$$

Therefore the electron spectrum is symmetrical about the band center $E = 0$. It follows hence that in (4.8) all $I_{2m+1} = 0$. Consequently Eq. (4.12) vanishes, and all that is left of the system (4.11) are $(q-1)/2$ equations with $k = q - 2m - 1$, where $1 \leqslant m \leqslant (q-1)/2$. Equations (4.12a) and (4.12c) are preserved, but now $s_1 = 0$ in (4.12c). By the same reasoning as used for model II, we find that in model I the H spectrum has three allowed bands, as shown in Fig. 1. The chemical potential is located in one of the two forbidden bands.

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The self-consistency equations (4.12a) and (4.12c) take the form

$$\varkappa = \frac{2}{\pi}\int_{E_1}^{E_2} E[-\bar{R}(E^2)]^{-1/2}dE, \qquad (4.20)$$

$$P = \frac{2}{\pi}\int_{E_1}^{E_2}\left(E^3 + \frac{s_2}{2}E\right)[-\bar{R}(E^2)]^{-1/2}dE, \qquad (4.21)$$

where

$$\bar{R}(E^2) = \prod_{i=1}^{3}(E^2 - E_i^2), \quad s_2 = -E_1^2 - E_2^2 - E_3^2.$$

As a consequence of (4.4), the state density is

$$\frac{2}{\pi}\frac{dp}{dE} = \frac{2}{\pi}[E^2 + C][-\bar{R}(E^2)]^{-1/2}, \qquad (4.22)$$

where the constant C is determined according to (4.5) from the condition

$$\int_{E_2}^{E_3}(E^2 + C)[\bar{R}(E^2)]^{-1/2}dE = 0. \qquad (4.23)$$

For the electron density ρ we obtain from (4.22), taking (4.23) into account

$$|\rho - 1| = \frac{1}{\pi}\int_{E_3}^{-E_3}(E^2 + C)[-\bar{R}(E^2)]^{-1/2}dE. \qquad (4.24)$$

In analogy with (4.19), the system length is expressed in terms of

$$I_0 = \lim_{E\to-\infty}\left[\ln E - \int_{E_1}^{E}(E^2 + C)[R(E^2)]^{-1/2}dE\right] = -a. \qquad (4.25)$$

The five equations (4.20), (4.21), (4.23)–(4.25) determine the three parameters E_i and the value of C, and yield the equation of state $P = P(a, \rho)$. The ground state energy is

$$w_0(a,\rho) = \frac{2}{\pi}\int_{E_1}^{E_2}E\frac{dp}{dE}dE + \varkappa I_2 = P - \frac{1}{2}\varkappa\left(C - \frac{1}{2}s_2\right). \qquad (4.26)$$

(At $s = 0$ we obtain from (4.16) $I_2 = -\varkappa s_2/2$.) We note that Eqs. (4.20)–(4.26) in Chap. 2 are written in the notation of the previously employed continual problem[6]:

$$-E_1 = E_m, \quad -E_2 = E_+, \quad -E_3 = E_-.$$

5. ELLIPTIC PARAMETRIZATION

1. The investigations of the equations derived in Chap. 4 can be simplified by introducing elliptic parametrization of the curve. In this parametrization it is possible also to obtain explicit equations for the distributions of x_n, c_n, v_n, ρ_n, and $\psi_n(E)$. Elliptic polarization is found to be particularly effective for model II, where it makes it possible in fact to solve the self-consistency equations (4.12). Just as in Chap. 4, we consider this model first.

For points on the Riemann surface Γ of the function $R^{1/2}(E)$

$$R(E) = \prod_{i=1}^{4}(E - E_i),$$

we introduce the parameter $z = z(E)$

$$z = \int_{E_1}^{E}R^{-1/2}(E')dE'. \qquad (5.1)$$
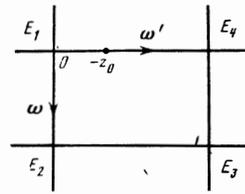

FIG. 5.

The half-periods of this elliptic integral are equal to

$$\omega = -\int_{E_1}^{E_2}R^{-1/2}(E)dE, \quad \omega' = -\int_{E_2}^{E_3}R^{-1/2}(E)dE. \qquad (5.2)$$

(The sign in front of the square root corresponds to the sheet containing the upper edge of the cut along which the integration is carried out.) Equation (5.1) establishes a one-to-one correspondence between the points of Γ and the z-plane points, apart from displacements by 2ω and $2\omega'$. Figure 5 shows for clarity the cell bounded by the half-periods ω and ω'.

The elliptic function $E(z)$ defined by (5.1) has poles at the points $\pm z_0$, where $z_0 = z(-\infty)$. The inversion of the integral (5.1) is given by[4]

$$E(z) = \zeta(z + z_0) - \zeta(z - z_0) + A,$$

where $\zeta(z)$ is the Weierstrass zeta function.[16] The parameters ω, ω', z_0, and A replace the parameters E_i in accord with Fig. 5:

$$E_1 = E(0), \quad E_2 = E(\omega),$$
$$E_3 = E(\omega + \omega'), \quad E_4 = E(\omega'). \qquad (5.2a)$$

We examine now the self-consistency equations expressed in terms of the new parameters. Equations (4.15) and (4.14) take the form

$$\rho = \frac{2}{\pi i}\int_0^\omega[E(z) + Q]dz = \frac{2}{\pi i}\left[\ln\frac{\sigma(z + z_0)}{\sigma(z - z_0)}\Big|_0^\omega\right.$$
$$\left. + (A + Q)\omega\right] = \frac{2}{\pi i}[\pi i + 2\eta z_0 + (A + Q)\omega], \qquad (5.3)$$

$$0 = \int_\omega^{\omega + \omega'}[E(z) + Q]dz = 2\eta'z_0 + Q\omega' + A\omega', \qquad (5.4)$$

$$z_0 = (\rho/2 - 1)\omega'. \qquad (5.5)$$

Equation (4.12a) determines ω:

$$\varkappa = 2i\omega/\pi. \qquad (5.6)$$

To use Eqs. (4.12b) and (4.12c) we must obtain expressions for s_1 and for $4s_2 - s_1^2$. We use for this purpose the following device. It is easy to verify that as $E \to \infty$ we have

$$[E^2 - \tfrac{1}{2}s_1 E + \tfrac{1}{2}(s_2 - \tfrac{1}{4}s_1^2)]R^{-1/2}(E) = 1 + O(E^{-3}).$$

The function $E(z)$ takes in the vicinity of $z = z_0$ the form

$$E(z) \approx -\frac{1}{z - z_0} + \zeta(2z_0) + A - \wp(2z_0)(z - z_0) + O(z - z_0)^2,$$

$$dE(z) = [\wp(z - z_0) - \wp(z + z_0)]dz = dz\left[\frac{1}{(z - z_0)^2} - \wp(2z_0) + \ldots\right].$$

Substituting these expressions in both halves of the preceding equation and comparing the first coefficients of the corresponding expansions, we get

$$s_1 = 4(\zeta_0 + A),$$
$$\tfrac{1}{8}s_1^2 - \tfrac{1}{2}s_2 = 3\wp_0 - (\zeta_0 + A)^2, \qquad (5.7)$$

where we have introduced for brevity the notation

$$\zeta_0 = \zeta(2z_0), \quad \wp_0 = \wp(2z_0), \quad 2z_0 = (\rho - 2)\omega'.$$

In addition, it follows from the same considerations that

$$dE\left[E^2 - \tfrac{1}{2}s_1 E + \tfrac{1}{2}s_2 - \tfrac{1}{8}s_1^2\right]R^{-1/2}(E) = [\wp(z - z_0) + \wp(z + z_0) - 2\wp_0]\,dz.$$

Indeed, both halves of these equations of single poles at $z = \pm z_0$, and have at these points the same values, accurate to $O(z \pm z_0)$.

From (4.12b) we can obtain A:

$$\int\limits_0^{\bullet}\left[E(z) - \frac{1}{2}s_1\right]dz = \pi i + 2\eta z_0 - (2\zeta_0 + A)\omega = 0. \tag{5.8}$$

Equation (4.12c) takes the form

$$P = \frac{2}{\pi i}\int\limits_0^{\bullet}[\wp(z - z_0) + \wp(z + z_0) - 2\wp(z_0)]\,dz = \frac{4}{\pi}i(\eta + \wp_0\omega). \tag{5.9}$$

It follows from (4.18) that

$$I_0 = \lim_{z \to z_0}\left[\ln E(z) - \int\limits_0^{z}[E(z') + Q]\,dz'\right]$$

$$= \lim_{z \to z_0}\left[\ln\left(-\frac{1}{z - z_0}\right) - \ln\left(\frac{\sigma(z + z_0)}{\sigma(z - z_0)}\right) - Qz_0 - Az_0\right] = 2z_0^2\frac{\eta'}{\omega'} - \ln[\sigma(-2z_0)],$$

or

$$I_0 = \tfrac{1}{2}\rho^2\eta'\omega' - \ln[\sigma(\rho\omega')]. \tag{5.10}$$

Given $\varkappa$ and ρ, Eqs. (5.5), (5.6), and (5.8) yield simple expressions for ω, z_0, and A. The half-period ω' parametrizes with the aid of (5.9) and (5.10) the equation of state of the system, be relating the pressure P to the average length $a = -I_0$.

From (4.19) follows an equation for the energy:

$$w_0 = P + \tfrac{1}{2}\varkappa\left[(\eta\omega'\rho/\omega - \eta' - \zeta(\omega'\rho))^2\right.$$
$$\left. - 3\wp(\omega'\rho)\right] + \rho(\eta\omega'\rho/\omega - \eta' - \zeta(\omega'\rho)). \tag{5.11}$$

Let us find the equilibrium values of x_n, c_n, v_n, and $\psi_n(E)$. The Bloch eigenfunction (relative to the period N) $\psi_n(z)$ of the operator H is a doubly periodic function that has according to Appendix 1 a pole of n-th order at the point $z = z_0$ and a zero of n-th order at the point $z = -z_0$. It has in addition a pole at the point $z = \alpha$ that corresponds to a certain point $E = \gamma$ in the forbidden band, and $\mathrm{Im}\,\alpha = \omega$.

The function $\psi_n(z)$, as any other elliptic function, can be expressed in terms of the Weierstrass σ function[16]:

$$\psi_n(z) = b_n\frac{\sigma^n(z + z_0)\sigma(z - \alpha_n)}{\sigma^n(z - z_0)\sigma(z - \alpha)}. \tag{5.12}$$

In order for $\psi_n(z)$ to be doubly periodic, it is necessary and sufficient for the sum of the zeros (with allowance for the multiplicity) of the numerator and of the denominator to be equal. Consequently

$$-nz_0 + \alpha_n = nz_0 + \alpha, \quad \alpha_n = 2nz_0 + \alpha = 2z_0(n - n_0) + \omega,$$

where n_0 are arbitrary but not necessarily rational numbers.

In the vicinity of the points $z = \pm z_0$ the function $\psi_n(z)$ takes the form

$$\psi_n(z) = \frac{b_n}{(z - z_0)^n}\sigma^n(2z_0)\frac{\sigma(z_0 - \alpha_n)}{\sigma(z_0 - \alpha)}\{1 + (z - z_0)[n\zeta(2z_0)$$
$$+ \zeta(z_0 - \alpha_n) - \zeta(z_0 - \alpha)] + O(z - z_0)^2\}, \quad z \to z_0;$$

$$\psi_n(z) = b_n\frac{(z + z_0)^n\sigma(-z_0 - \alpha_n)}{\sigma^n(-2z_0)\sigma(-z_0 - \alpha)}, \quad z \to -z_0. \tag{5.12a}$$

On the other hand, according to Eq. (A1.4),

$$\psi_n = \exp(x_n)E^n[1 + \xi_1(n)E^{-1} + O(E^{-2})],$$
$$\psi_n = \exp(-x_n)E^{-n}[1 + O(E^{-1})]. \tag{5.12b}$$

Comparing the expansions of (5.12a) and (5.12b) we obtain

$$\exp(2x_n) = \sigma^{2n}(-2z_0)\frac{\sigma(z_0(1 - 2n) - \alpha)\sigma(z_0 + \alpha)}{\sigma(z_0(1 + 2n) + \alpha)\sigma(z_0 - \alpha)}, \tag{5.13a}$$

$$v_n = \xi_1(n) - \xi_1(n + 1) = 2\zeta(2z_0) + A$$
$$+ \zeta((2n - 1)z_0 + \alpha) - \zeta((2n + 1)z_0 + \alpha). \tag{5.13b}$$

2. **Model I.** Equations (4.20)–(4.26) of model I can also be written in terms of elliptic functions. In this case, however, it is necessary to use elliptic functions with different pairs of periods.

We set each point of the Riemann surface of the function $R^{1/2}(E^2)$

$$R(E^2) = (E^2 - E_1^2)(E^2 - E_2^2)(E^2 - E_3^2),$$

in correspondence with a pair of complex numbers

$$z_1 = \int\limits_{E_1}^{E}R^{-1/2}(E^2)\,dE, \quad z_2 = \int\limits_{E_1}^{E}ER^{-1/2}(E^2)\,dE. \tag{5.14}$$

We define the half-periods

$$\omega_1 = \int\limits_{E_1}^{E_2}R^{-1/2}(E^2)\,dE, \quad \omega_1' = \int\limits_{E_2}^{E_3}R^{-1/2}(E^2)\,dE;$$

$$\omega_2 = \int\limits_{E_1}^{E_2}ER^{-1/2}(E^2)\,dE, \quad \omega_2' = \int\limits_{E_2}^{E_3}ER^{-1/2}(E^2)\,dE.$$

(The integration is over the lower sheet or along the upper edge of the cut of the lower sheet).

The integrals (5.14) map the surface Γ on the basic cells of lattices with periods $(2\omega_1, 2\omega_1')$, $(2\omega_2, 2\omega_2')$, see Figs. 6a and 6b. Both integrals in (5.14) can be reduced to elliptic by the substitution $y = E^2$. We consider the first of them:

$$z_1 = \frac{1}{2}\int\limits_{E_1^2}^{E^2}(yR(y))^{-1/2}\,dy.$$

The inversion of such an integral was considered at the beginning of this chapter. We obtain

$$E^2(z_1) = \tfrac{1}{2}[\zeta(z_1 + z_{10}) - \zeta(z_1 - z_{10})] + B, \tag{5.15}$$

$$z_{10} = \frac{1}{2}\int\limits_{E_1^2}^{\infty}(yR(y))^{-1/2}\,dy.$$

The parameters ω_1, ω_1' and z_0 replace E_i^2. Since one of the branch points of the function $(yR(y))^{1/2}$ is zero, the corresponding mapping (see Fig. 6a) determines B:
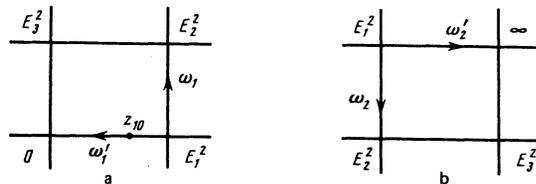

FIG. 6.

$$E^2(\omega_i')=0=B+\zeta(z_{10})+\wp'(z_{10})/2[\wp(z_{10})-\wp(\omega_i')]. \qquad (5.16)$$

So far, the Weierstrass ζ and $\wp$ functions were determined by the half-periods ω_1 and ω_1'. We shall next use together with them also functions made up of the half-periods ω_2 and ω_2'. The differences between the corresponding functions will be identified by the subscript of the argument. For example,

$$\zeta(z_1)=\zeta(z_1, \omega_1, \omega_1'), \quad \zeta(z_2)=\zeta(z_2, \omega_2, \omega_2')$$

and so forth.

The inversion of the integral (5.14)

$$z_2(E^2)=\frac{1}{2}\int_{z_1^2}^{E^2} R^{-1/2}(y)\,dy$$

is given by the formula[16]

$$E^2(z_2)=\wp(z_2-\omega_2')+A,$$
$$E^2(0)=E_1^2, \quad E^2(\omega_2)=E_2^2, \quad E^2(\omega_2+\omega_2')=E_3^2. \qquad (5.17)$$

The connection between the two parametrizations (5.15) and (5.17), i.e., between the three triplets of parameters ω_1, ω_1', z_{10} and ω_2, ω_2', and A can be obtained by equating the values of $E^2(z_1)$ and $E^2(z_2)$ in the corresponding half-periods. With allowance for (5.16) we have

$$E_1^2=\wp(\omega_2')+A=\wp'(z_{10})/2[\wp(\omega_i')-\wp(z_{10})], \qquad (5.18a)$$
$$E_1^2-E_2^2=\wp(\omega_2')-\wp(\omega_2-\omega_2')=\wp'(z_{10})/2[\wp(\omega_i)-\wp(z_{10})], \qquad (5.18b)$$
$$E_1^2-E_3^2=\wp(\omega_2')-\wp(\omega_2)=\wp'(z_{10})/2[\wp(\omega_i+\omega_i')-\wp(z_{10})]. \qquad (5.18c)$$

Since

$$\wp(\omega_2)+\wp(\omega_2')+\wp(\omega_2-\omega_2')=0,$$

it follows that

$$-s_2=E_1^2+E_2^2+E_3^2=3A.$$

In analogy with (5.7a) we have

$$-s_2=2\zeta(2z_{10})+4B.$$

Using (3.16), we obtain

$$3A=2\zeta(2z_{10})-4\zeta(z_{10})+2\wp'(z_{10})/[\wp(\omega_i')-\wp(z_{10})]. \qquad (5.19)$$

Equations (4.20) and (4.21) take in the new parametrization the form

$$\varkappa=2i\omega_2/\pi, \qquad (5.20a)$$

$$P=\frac{2}{\pi i}\int_0^{\omega_i}\left[E^2(z_2)+\frac{1}{2}s_2\right]dz_2=\frac{2i}{\pi}\left(\zeta(\omega_2)+\frac{1}{2}A\omega_2\right)$$
$$=\frac{2i}{\pi}\left\{\zeta(\omega_2)+\frac{\omega_2}{3}\left[\zeta(2z_{10})-2\zeta(z_{10})+\frac{\wp'(z_{10})}{\wp(\omega_i')-\wp(z_{10})}\right]\right\}. \qquad (5.20b)$$

The differential of the quasimomentum is

$$idp=(E^2+C)dz_1=[1/2\zeta(z_1+z_{10})-1/2\zeta(z_1-z_{10})+B+C]dz_1.$$

The constant C is determined by the normalization condition

$$0=\int_{\omega_i}^{\omega_i+\omega_i'}dp=\frac{1}{2}\ln\frac{\sigma(z_1+z_{10})}{\sigma(z_1-z_{10})}\Big|_{\omega_i}^{\omega_i+\omega_i'}+(B+C)\omega_i',$$

or

$$B+C=-\eta_1'z_{10}/\omega_i'.$$

Equation (4.25) yields

$$z_{10}=-|\rho-1|\omega_i'. \qquad (5.20c)$$

Equation (4.27) yields

$$I_0=\lim_{z_1\to z_{10}}\left[\ln E(z_1)-\frac{1}{2}\ln\frac{\sigma(z_1+z_{10})}{\sigma(z_1-z_{10})}-(B+C)z_{10}\right]$$
$$=-\frac{1}{2}\ln[2\sigma(-2z_{10})]+\eta_1'\frac{z_{10}^2}{\omega_i'}.$$

Substituting (5.20c), we obtain ultimately

$$a=-I_0={}^1/_2\ln[2\sigma(2|\rho-1|\omega_i')]-(\rho-1)^2\eta_1'\omega_i'. \qquad (5.21)$$

Expression (4.26) for the energy of the ground state can now be written in the form

$$w_0=P+\frac{\varkappa}{2}\left\{\zeta(2|\rho-1|\omega_i')-\zeta(|\rho-1|\omega_i')-\eta_1'|\rho-1|\right.$$
$$\left.+\frac{\wp'(|\rho-1|\omega_i')}{2[\wp(\omega_i')-\wp(|\rho-1|\omega_i')]}\right\}. \qquad (5.22)$$

The square of the Bloch (relative to the period N) function ψ_n^2 is an even function on the Riemann surface Γ relative to the transformation $E, \Lambda \to -E, (-1)^N\Lambda$ or, equivalently, relative to the transformation $E, R^{1/2} \to -E, -R^{1/2}$. Consequently ψ_n^2 is a function of only the coordinate z_1. The analytic properties of ψ_n^2 yield lead, in analogy with (5.12), to the expression

$$\psi_n^2(z_1)=\frac{b_n}{\sigma^2(z_1-\alpha)}\frac{\sigma^n(z_1+z_{10})}{\sigma^n(z_1-z_{10})}\begin{cases}\sigma^2(z_1-\alpha_n), & n=2m, \\ \sigma(z_1-\alpha_n-\omega_1')\sigma(z_1-\alpha_n+\omega_1'), & n=2m+1\end{cases}$$

where $\alpha_n=nz_{10}+\alpha=|\rho-1|(n_0-n)\omega_1'+\omega_1$. $\qquad (5.23)$

We recall once more that in the vicinity of $z_1=\pm z_{10}$

$$E^2(z_1)=\pm 1/2(z\pm z_{10}),$$

and the function ψ_n^2 itself has the asymptotic form

$$\psi_n^2=\exp(\pm 2x_n)E^{\pm 2n}+O(E^{\pm 2n-1}).$$

Comparing the last formula with the coefficients of the leading terms in the expansion (5.23) in the vicinity of $z=\pm z_{10}$, we get

$$\exp 2x_n=[2\sigma(-2z_{10})]^n\frac{\sigma(z_{10}+\alpha)}{\sigma(z_{10}-\alpha)}$$
$$\times\begin{cases}\sigma(z_{10}(1-n)-\alpha)\sigma^{-1}(z_{10}(1+n)+\alpha), & n=2m, \\ \sigma(z_{10}(1-n)-\alpha-\omega_1')\sigma^{-1}(z_{10}(1+n)+\alpha+\omega_1'), & n=2m+1.\end{cases} \qquad (5.24)$$

From Eqs. (A1.6) and (A1.7) we obtain for the charge density

$$\rho_n=1+\text{sign}(\rho-1)\left\{1-\frac{2}{\pi i}\int_0^{\omega_i}[E^2(z_1)-E^2(nz_{10}+\alpha)]dz_1\right\},$$

$$\rho_n=1+\text{sign}(\rho-1)\frac{2}{\pi i}\left\{\eta_1\omega_i'|\rho-1|+\frac{1}{2}\omega_i[\zeta(-(n+1)|\rho-1|\omega_i'+\alpha)\right.$$
$$\left.-\zeta(-(n-1)|\rho-1|\omega_i'+\alpha)]\right\}. \qquad (5.25)$$

APPENDIX 1

In this Appendix we consider the analytic properties of the functions $\psi_n(E)$, and obtain expressions for the variations δp of the momentum and of the state density dp/dE.

To each pair (Λ, E) satisfying Eq. (4.1) there corresponds a unique solution ψ_n of Eq. (1.1), which is an eigensolution for the shift operator $\psi_{n+N}=\Lambda\psi_n$ and is normalized by the condition $\psi_0=1$. We call this a Bloch solution (relative to the period N). The vector

$(\psi_0, \psi_1) = (1, \psi_1)$ is an eigenvector for the matrix T, hence

$$\psi_n = \varphi_n(E) + [\Lambda - \varphi_N(E)] \theta_N^{-1}(E) \theta_n(E). \tag{A1.1}$$

At each value of E (other than those for which $Q^2(E) = 1$) there are two Bloch functions corresponding to different solutions of Eq. (4.1). The Bloch function is single-valued on the algebraic curve Γ of the function $[Q^2(E) - 1]^{1/2}$. As $E \to \infty$ the Bloch function has two asymptotic forms $\psi_n^{(\pm)}(E)$ on two sheets of the surface Γ which correspond to the two roots of Eq. (4.1):

$$\Lambda_\pm = Q(E) \pm Q(E)[1 + O(E^{-2N})].$$

It is easy to verify that

$$\psi_n^{(\pm)}(E) = \tilde{b}_n^{(\pm)} E^{\pm n} \left[1 + \sum_{k=1}^{\infty} \xi_k^{(\pm)} E^{-k}\right], \tag{A1.2}$$

i.e., $\psi_n(E)$ has a pole of order n on one sheet and a zero of order n on the other.

Away from infinity, $\psi_n(E)$ is analytic on Γ everywhere except at the points $E = \gamma$ at which $\theta_N(\gamma) = 0$, where $\psi_n(E)$ has poles. Since $\theta_N(\gamma) = 0$, we have

$$\varphi_N(\gamma) \theta_{N+1}(\gamma) = \det T = 1.$$

Consequently

$$|Q(\gamma)| = \tfrac{1}{2} |\varphi_N(\gamma) + \theta_{N+1}(\gamma)| \geq 1, \tag{A1.3}$$

i.e., the poles γ of the function $\psi_n(E)$ lie in forbidden bands. We note that $\psi_n(E)$ has a pole only on one sheet above the point γ. Indeed, since $\theta_n(\gamma) = 0$, one of the roots of (4.1) equals $\varphi_N(\gamma)$. Corresponding to this root is a finite value $\bar\psi_n$, since the zeros of the numerator and denominator of the second term of (A1.2) cancel out. It is easy to deduce from (A1.2) that $\psi_n(E)$ has no singularities at the band-merging points. Thus, for any operator H with periodic coefficients the Bloch function ψ_n is a single-valued function on the Riemann surface Γ. It is analytic everywhere on this surface except at the points γ_s, $1 \leq s \leq N - 1$, one over each forbidden band. Substituting (A1.2) in (1.1) and (1.4) we easily find that

$$\tilde{b}_n^{(\pm)} = \exp(\pm x_n), \quad \xi_1^{(+)}(n) - \xi_1^{(+)}(n+1) = v_n. \tag{A1.4}$$

The converse is also true. Any set of E_i and of the points γ_i determines uniquely the coefficients c_n and v_n of the (generally speaking quasiperiodic) operator H.[19] Explicit expressions for c_n and v_n in terms of E_i and γ_i, in which Riemann theta functions are used, can be found in Ref. 19.

Let ψ_n and ψ_n' be the Bloch functions for the operators H and H'

$$c_n \psi_{n+1} + v_n \psi_n + c_{n-1} \psi_{n-1} = E \psi_n,$$
$$c_n' \psi_{n+1}' + v_n' \psi_n' + c_{n-1}' \psi_{n-1}' = E \psi_n'.$$

We multiply the first equation by ψ_n' and the second by ψ_n, and subtract one from the other. Summing the obtained expressions over n, we have

$$c_{N-1}(\psi_N' \psi_{N-1} - \psi_N \psi_{N-1}')[1 - \Lambda^{-1}(\Lambda')^{-1}]$$
$$= \sum_{n=0}^{N-1} \delta v_n \psi_n \psi_n' + (\psi_{n+1}' \psi_n + \psi_n' \psi_{n+1}) \delta c_n, \tag{A1.5}$$
$$v_n' = v_n + \delta v_n, \quad c_n' = c_n + \delta c_n.$$

Accurate to terms of first order it can be assumed that ψ_n' is the solution of the equation $H\psi_n' = E\psi_n'$. We use for ψ_n' not ψ_n, but the value $\bar\psi_n$ of ψ_n on the second sheet of the surface Γ. We note that $\bar\psi_n = \psi_n^*$ in the allowed band. With this choice of ψ_n' we have

$$1 - \Lambda^{-1}(\Lambda')^{-1} = 1 - \exp[i(p' - p)N] \approx -i\delta pN.$$

The coefficients of δv_n and δc_n in (A1.5) are symmetric functions independent of interchange of the sheets. They are therefore rational functions of E and have poles at the points γ_i. It follows from (A1.3) that as $E \to \infty$ we have

$$\psi_n \bar\psi_n \to 1, \quad \psi_{n+1} \bar\psi_n + \psi_n \bar\psi_{n+1} \to E + O(E^{-1}).$$

Thus,

$$\psi_n \bar\psi_n = \prod_{i=1}^{q}(E - \gamma_i(n)) \Big/ \prod_{j=1}^{q}(E - \gamma_j),$$

$$\psi_{n+1} \bar\psi_n + \psi_n \bar\psi_{n+1} = P_n(E) \prod_{i=1}^{q}(E - \gamma_i)^{-1}. \tag{A1.6}$$

Here $\gamma_i(n)$ are the projections of the zeros of ψ_n, and P_n is a polynomial of degree $q + 1$.

The function $c_{N-1}(\bar\psi_N \psi_{N-1} - \psi_N \bar\psi_{N-1})$ is odd with respect to interchange of the sheets, has poles over the points ψ_i, and tends on the upper sheet to $-E$ as $-E \to \infty$. This function is therefore equal to

$$c_{N-1}(\bar\psi_N \psi_{N-1} - \psi_N \bar\psi_{N-1}) = -R^{1/2}(E) \prod_{i=1}^{q}(E - \gamma_i)^{-1}.$$

Substitution of the obtained expressions in (A1.5) yields expression (4.7) for δp. In analogy with the derivation of (A1.5) we obtain by varying the coefficients of H rather than of E

$$dE \left(\sum_{n=0}^{N-1} \psi_n \bar\psi_n\right) = c_{N-1}(\bar\psi_N \psi_{N-1} - \bar\psi_{N-1} \psi_N)[1 - \Lambda^{-1}(\Lambda')^{-1}]$$

$$= [R(E)]^{1/2} \prod_{i=0}^{q}(E - \gamma_i(n))^{-1} iN dp,$$

or

$$i \frac{dp}{dE} = N^{-1}[R(E)]^{-1/2} \sum_{n=0}^{N-1} \prod_{i=0}^{q}(E - \gamma_i(n)). \tag{A1.7}$$

For model II, comparison of (A1.6) at $q = 1$ with (5.12) shows that $\gamma_1 = E(\alpha_n)$. For model I, comparison of (A1.6) at $q = 2$ with (5.23) shows that $\gamma_1 = -\gamma_2 = E^2(\alpha_n)$.

APPENDIX 2

It will be proved below that there are no more than three allowed bands for the operators H that are extremal with respect to the functional (1.5).

We consider the variation of the first part of the functional (1.5). Since the energy levels E in the allowed bands are roots of the polynomial $Q(E) - 1$, we have

$$\frac{1}{N} \sum \delta E = - \sum_E \text{res} \frac{\delta Q}{N(Q-1)}, \tag{A2.1}$$

where res_E denotes the residue at the point E. We denote by $R_\pm$ and $r_\pm$ polynomials that vanish respectively

in the simple and doubly degenerate roots of the polynomials $Q \mp 1$, i.e.,

$$Q \mp 1 = a_{\pm} R_{\pm} r_{\pm}^2, \quad R_{+} R_{-} = R(E), \quad (A2.2)$$

where $a_{\pm}$ are constants. The edges of the allowed bands coincide with the simple roots of the polynomial $Q^2(E) - 1$, i.e., with the roots of the polynomial $R(E)$. We denote the degree of R by $2q + 2$. We express the variation δp in analogy with the differential (4.4) and compare with (4.7) and (4.9). Taking (A2.2) into account we get

$$N^{-1} \delta Q = r_{+}(E) r_{-}(E) \sum_{k=0}^{q+1} l_k E^{q+1-k}. \quad (A2.3)$$

With the aid of (A2.1) and (A2.3) we can express the equation for the extremals of the functional (1.5) in the form

$$0 = \delta W = \varkappa \delta I_2 - P \delta I_0 - \sum_{E < \mu} \operatorname{res}_E r_{-}(E) r_{+}^{-1}(E) R_{+}^{-1}(E) \sum_{h=0}^{q+1} l_k E^{q+1-h}. \quad (A2.4)$$

Since all three differentials δI_s with $s \leq q + 1$ are linearly independent, we obtain, equating to zero the coefficients of δI_s with $3 \leq s \leq q + 1$,

$$\sum_{E < \mu} \operatorname{res}_E \frac{E^k r_{-}(E)}{R_{+}(E) r_{+}(E)} = 0, \quad k \leq q - 2. \quad (A2.5)$$

Without loss of generality we can assume that there are no less than $[q/2]$ forbidden bands to the left of μ. In the opposite case we can change over in (A2.5) to summation over $E > \mu$, since the sum of all the residues of the function $E^k r_{-} r_{+}^{-1} R^{-1}$ is zero at $k \leq q - 2$.

Let μ_s be arbitrary points each in one forbidden band to the left of E_m. Then

$$\sum_{i=1}^{m} \operatorname{res}_{E_i} \prod_{s=1}^{[q/2]} (E - \mu_s) r_{-}(E) r_{+}^{-1}(E) R_{+}^{-1}(E) \neq 0. \quad (A2.6)$$

Let us prove the last statement. By definition, the polynomial $R_{+} r_{+}$ has simple roots. Consequently, in neighboring points the signs of the residues are opposite. From the definition of the allowed bands it is seen that a double root of the polynomial $Q + 1$, or a root r_{-}, must be located between neighboring roots $R_{+} R_{+}$ located in the same band. Thus, in each of the allowed bands all the residues of the function $r_{-} R_{+}^{-1} r_{+}^{-1}$ have the same sign that is reversed on going to the neighboring band. The sign of $\Pi_s (E - \mu_s)$ varies similarly, thereby proving (A2.6).

Equation (A2.6) contradicts (A2.5) if $[q/2] \leq q - 2$. It follows therefore that $q \leq 2$ (for otherwise the preceding inequality will be satisfied).

APPENDIX 3

The end purpose of this Appendix is to prove that in the ground state of the system considered the chemical potential must be located in one of the forbidden bands. As already mentioned in Chap. 4, this means that the electron spectrum has in the ground state a single band.

The derivation of the self-consistency equations (4.11) and (4.12) for the functional (1.5) was quite general and can be readily extended to the case when the system energy depends not only on the first integrals I_0 and I_2,

but also on some number of higher integrals, e.g.,

$$W = \frac{2}{\pi} \int_{E_1}^{\mu} dp - P I_0 + \sum_{j=1}^{r} \varkappa_j I_j.$$

Since the upper bound on the number of bands increases in this case, $q \leq 2r - 2$, we shall discuss hereafter the system (4.11), (4.12) for the general case, without using the condition $q \leq 2$.

Equations (4.11) and (4.12) (or their analogs) are the necessary and sufficient conditions for the functional $\tilde{W}$ to be extremal in the considered class of the periodic operators H. The number of these equations is $q + 2$. The periodicity of the operator H is equivalent to $q + 1$ equations (4.6), we have therefore a total of $2q + 3$ equations for the $2q + 3$ unknowns $E_1, \ldots, E_{2q+2}, \mu$. The equations (4.11) and (4.12) are thus the conditions that $\tilde{W}$ be extremal at a fixed set of numbers $\rho_k = m_k / N$, which can assume arbitrary rational values as $N \to \infty$.

To compare the values of $\tilde{W}$ for different sets of ρ_k, we proceed as if we had to minimize a function specified only on a set of rational points. The minimum of such a function can be easily obtained if it is possible to construct a smooth function that coincides with the considered one at the rational points. In our case such a smooth function was in fact already constructed. Let us formulate this more distinctly.

For any set $E_1 < \ldots < E_{2q+2}$ there exists a unique differential dp given by

$$i \, dp = R^{-1/2}(E) \left[E^q + \sum_{j=0}^{q-1} a_j E^{q-j} \right] dE,$$

and normalized by the conditions (4.5). We define $I_k(E_i)$ by Eq. (4.8).

Since we have it in mind to vary subsequently the numbers ρ_k, it is natural to admit also of variation of the total number of electrons

$$N_e = \sum \rho_k$$

and use the functional

$$\Omega(E_i) = \frac{1}{\pi} \int_{E_1}^{\mu} E \, dp + \varkappa I_2(E_i) - P I_0(E_i) - \mu N_e$$

at fixed μ. This functional can be considered at all, not necessarily "rational," sets of E_i. The variations δp are then no longer single-valued on Γ. A variation becomes single-valued if Γ is cut also along the cycles above the forbidden band. Each integral with respect to E from E_1 to μ, which we used above, must be understood here not as a sum of integrals over the allowed bands, but as half the value of the integral over a cycle that begins at μ on the lower edge of the cut and returns to μ around E_1 along the upper edge. Variations for which

$$\int_{E_{2k-1}}^{E_{2k}} dp = \text{const},$$

are called variations that conserve the group of periods of the differential dp. With respect to these variations, the differential $d(\delta p)$ has null periods over all the cycles. Consequently the function $\delta p = \int dp$ is single-valued on the surface Γ. Since it is odd with respect

to interchange of the sheets, it must be of the form (4.7). Equations (4.12) and (4.11) coincide with the extremum equations with respect to variations that preserve the group of periods.

For general variations of the set $\{E_i\}$ the function δp is no longer unique on Γ. It becomes unique if Γ is cut along the cycles above the forbidden bands. The function δp has poles at the edges of the bands, and undergoes on the cuts along the k-th forbidden bands a discontinuity equal to

$$\delta\rho_k = \int_{E_1}^{E_{2k}} d\delta p.$$

If Γ were to be an ordinary complex plane, the function having a specified discontinuity on some arbitrary contour would be expressed in standard fashion with the aid of a Cauchy integral. The general problem of constructing a piecewise meromorphic function of arbitrary algebraic curves is called the Riemann problem and is the subject of an extensive literature (see the review[20]). Without going into details of this theory, we can in our case write down directly an answer that lends itself to simple verification

$$i\delta p = \sum_{j=0}^{q+1} l_j E^q R^{-1/2}(E) + \frac{1}{2\pi} \sum_{k=1}^{q} \delta\rho_k \int_{E_{2k}}^{E_{2k+1}} \left(\frac{R(t)}{R(E)}\right)^{1/2} \frac{dt}{E-t}. \quad (A3.1)$$

It is easily seen that this function has poles only at the edges of the bands. Since the integrand tends as $E \to t$ to the Cauchy kernel $(E-t)^{-1}dt$ it follows that $i\delta p$ has the required discontinuities on the cuts. Expanding (A3.1) in the vicinity of $E = \infty$ and comparing with the expansion (4.8), we find that δI_k are linear combinations of l_i and $\delta\rho_k$. In turn, l_i and $\delta\rho_k$ are linearly expressed in terms of δI_k with $0 \leq k \leq 2q$, and Eqs. (4.9) hold for l_i. The independent differentials with respect to all the variations of the band edges are δI_k with $0 \leq k \leq 2q$. It is more convenient to choose as the independent differentials combinations that coincide with $\delta\rho_k$, as well as the differentials δI_s with $0 \leq s \leq q+1$. Then, varying Ω, we obtain in analogy with (4.10)

$$\delta\Omega(E_i) = \sum_{k=0}^{q+1} A_k \delta I_k + \sum_{k=1}^{q} B_k \delta\rho_k.$$

Setting the coefficients A_k equal to zero we get (4.11) and (4.12). It is necessary to add to them the equations $B_k = 0$, or

$$\int_{E_1}^{\mu} R^{-1/2}(E)\,dE \int_{E_{2k}}^{E_{2k+1}} (E-t)^{-1} R^{1/2}(t)\,dt = 0. \quad (A3.2)$$

As proved in Chap. 4, it follows even from (4.11) and (4.12) that for the extremals we always have $q \leq 2$, and $q = 2$ can occur only if μ lies in the central allowed band. We consider the case $q = 1$ and assume that μ does not lie in the forbidden band (E_2, E_3). In this case there is one additional condition (A3.2) at $k = 1$. This equation, obviously, has no solutions. If $\mu < E_2$, the integrand has a constant sign on the interval (E_1, μ). If $\mu > E_3$, we must consider the equivalent equation with an integral over the region $E > \mu$. Consequently, at $q = 1$ the chemical potential μ is located in the forbidden band, $E_2 < \mu < E_3$. Equations (A3.2) determine the chemical potential in the case when the latter is in the forbidden band. At $q = 1$ we have

$$\int_{E_1}^{\mu} \frac{dE}{R^{1/2}(E)} \int_{E_2}^{E_3} \frac{R^{1/2}(t)\,dt}{E-t} = 0.$$

Recalling the given definition of the integral with respect to E as an integral over the cycle (μ, E_1), we rewrite this equation in the form

$$\int_{E_1}^{E_2} \frac{dE}{R^{1/2}(E)} \int_{E_2}^{E_3} \frac{R^{1/2}(t)\,dt}{E-t} + \pi i (\mu - E_2) = 0.$$

It is easily verified that this equation has a root precisely at $E_2 < \mu < E_3$. We note for this purpose that the integral with respect to E in (A3.2), taken over the full cycle from E_1 to E_4, is zero. The imaginary part of the integral increases (decreases) with increasing distance from μ to E_1 and decreases (increases) with increasing distance from μ to E_2 along one of the edges of the cut.

We ultimately have

$$\mu = E_2 + \frac{1}{\pi} \int_{E_1}^{E_2} \frac{dE}{|R(E)|^{1/2}} \int_{E_2}^{E_3} \frac{|R(t)|^{1/2}\,dt}{t-E}. \quad (A3.3)$$

[1] For a verification of the self-consistent-field method and a discussion of the extremum conditions see Refs. 6 and 12. We note that the eigenvalue equation (1.1) is the condition for the extremum of the energy functional with respect to the wave functions ψ_n.

[2] The designations E_+ and E_- for the band boundaries correspond to the designations of the previously investigated[6] continual model. The upper limit E_m of the electron spectrum was treated in Ref. 6 as the cutoff energy of the linear spectrum.

[3] Here and elsewhere, where the limits of the integrals with respect to E are not explicitly indicated, it is assumed that the integration is over all the allowed bands contained in the indicated region ($E < \mu$ or $E > \mu$).

[4] For the rules for expressing an arbitrary elliptic function in terms of standard Weierstrass functions see Ref. 16.

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