THE COMMENSURABILITY ENERGY OF SOLIDS

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The energy difference between the commensurable (periodic) and incommensurable (almost-periodic) structures of a solid (the so-called commensurability energy) is calculated for a one-dimensional model of solid with finite-gap potential.

1. Introduction

It is well known that all solids are built of electrons and nuclei and the nuclei form a structure of the solid. We classify solids by a character of this structure. If the nuclei are arranged in a lattice the solid is a crystal; if the nuclei are arranged randomly, the solid has an amorphous structure. We can consider the above two structures as the limit cases of almost-periodic structures. Hence it looks reasonable to classify the solids as periodic solids (or crystals), random (or amorphous) solids and properly almost-periodic solids. Such a classification of solids was proposed for the first time in [1, 2].

A solid is characterized by a free energy F which depends on a structure. The equilibrium structure is defined by an equation $\delta F/\delta u(x) = 0$ where $u(x)$ is a potential created by the structure. An aim of our paper is to calculate a commensurability energy,

$$\Delta F = F^{(a)} - F^{(p)},$$

where $F^{(p)}, F^{(a)}$ are free energies of periodic and almost-periodic structures respectively. Therefore the commensurability energy defines whether a solid is periodic or almost-periodic. And this fact is very important because many physical properties of these classes of solids differ essentially. In our paper, we propose a consistent and rigorous approach to the problem of calculation of the commensurability energy of solid with a finite-gap structure.

The paper is organized as follows. In Section 1, we describe the almost-periodic structures and their properties. Section 2 is devoted to the description of finite-gap potentials. In Section 3, we calculate the averages for periodic and almost-periodic structures and compare them. In Section 4, we calculate the commensurability energy of a solid with a one-dimensional finite-gap structure in terms of averages for the periodic and ergodic cases.

2. Almost-periodic Solids and Their Properties

The theory of almost-periodic functions was created mainly by H. Bohr in the 1920s. For simplicity, we consider further only one-dimensional almost-periodic functions, a generalization of results for many-dimensional case being straightforward.

Among many possible definitions of almost-periodic functions, we choose the following one. A function $f(x)$ is called almost-periodic if it is a uniform limit of trigonometric polynomials, i.e. for any $\varepsilon > 0$, there exists such a trigonometric polynomial $P_{n(\varepsilon)}(x)$ of the $n(\varepsilon)$-th order that $\sup_{x\in\mathbb{R}} |f(x) - P_{n(\varepsilon)}(x)| < \varepsilon$.

The properties of an almost-periodic function $f(x)$ depend essentially on the basis of its Fourier frequencies. If the basis of Fourier frequencies is integer and one-dimensional then the almost-periodic function is periodic one. If the basis of Fourier frequencies is integer and finite, then the almost-periodic function is called a quasi-periodic one and may be considered as a value on the diagonal of some periodic function of a finite set of variables. To classify quasi-periodic functions, we must use many-dimensional crystallographic groups.

The properly almost-periodic structure of nuclei is a common object in the physics of solids: a vibrating lattice at a fixed moment of time forms an almost-periodic arrangements of nuclei. If this arrangement is stabilized by means of any physical reasons, then it becomes an equilibrium structure. We should only remember that there exists a lot of various types of waves in a solid: charge density waves, magnetic (or spin) density waves, concentration waves, etc. All these waves may have incommensurable periods. Thus, the almost-periodicity in solids has various physical manifestations.

Today physicists know hundreds of properly almost-periodic solids and we mention a few of them.

First of all, we should mention the solids with charge density waves. Among them, there

are quasi-one-dimensional (e.g., organic complexes with charge transfer, similar to tetrathiofulvalene tetracyanquinodimethane TTF—TCNQ; plane square complexes of transition metals with intermediate valence, similar to the salt $K_2Pt(CN)_4Br_{0.3}\ 3H_2O$, abr. KCP; trichalcogenides of transition metals with the chemical formula TX_3, where T means a transition metal such as Nb, Ta, and Ti, and X means chalcogen S, Se, Te; polyacetylene, etc.), quasi-two-dimensional (e.g., dichalcogenides of transition metals), three-dimensional (e.g., intermetallic compounds built of transition metals with the structure $A-15$ similar to that of Nb_3Sn). For a long time, we know magnetics with incommensurable arrangements of charge and magnetization: e.g., chromium and some alloys on its basis, numerous rare earth metals with spiral magnetic structures with periods depending on temperature and pressure. In ordering alloys, we meet various types of concentration waves. Quasi-crystals, which were discovered in 1984 [3], are quasi(and therefore almost)-periodic solids.

In order to understand the physical properties of almost-periodic solids, we must study spectral properties of the Schrödinger operator with almost-periodic potential. These studies were initiated by G. Scharf [4], E.D. Belokolos [1], Ya.G. Sinai and E. Dinaburg [5].

The Schrödinger operator with continuous almost-periodic potential is self-adjoint. For this operator we can prove the existence of the number of states (or the integrated density of states) $N(E)$ and other similar thermodynamic limits of spectral characteristics, e.g. the Fermi energy.

The number of states $N(E)$ is a non-decreasing function of the energy E and is defined by the following expression true everywhere besides the points of discontinuity:

$$N(E) = \lim_{|V_k|\to\infty} |V_k|^{-1} N_{V_k}(E). \qquad (1)$$

Here V_k is a bounded domain in $\mathbb{R}^d$ with the Lebesgue measure $|V_k|$ and $N_{V_k}(E)$ is the standard distribution function of a discrete spectrum in the domain V_k with some self-adjoint boundary conditions (Shubin, [6]). This statement is a direct consequence of the existence of the mean value of the potential which is a general property of all almost-periodic functions.

It appears that the spectrum $\sigma(H)$ of a Schrödinger operator with almost-periodic potential is essential, i.e. it does not contain isolated eigenvalues of finite multiplicity. We know a character of the spectrum for Schrödinger operators with almost-periodic potential in the limit cases: the spectrum of a Schrödinger operator with periodic potential is absolute continuous and the spectrum of a Schrödinger operator with random potential is point. It appears that, in general case, the spectrum of a one-dimensional Schrödinger operator with almost-periodic potential may have point, absolutely continuous, and singular continuous parts.

We can also label the gaps of the spectrum by the elements of the frequency module of an almost-periodic potential, similar to that as it has place for a periodic one. For the Schrödinger operator with the continuous almost-periodic potential $u(x)$ and the energy $E \in \mathbb{R}\backslash\sigma(H)$ the number of states $N(E) \in \Omega_u$, where Ω_u is the frequency module of the almost-periodic potential $u(x)$ (Belokolos, [1]; Johnson and Moser, [7]).

The class of almost-periodic solids has many interesting physical properties, which makes these solids very important from the point of view of possible practical applications. The almost-periodic solids can be conductors and dielectrics, they can have boundaries of mobility in the electron spectrum which separate the point and absolute continuous components of the spectrum, they can have the Cantor type spectrum (or the singular continuous type spectrum). In the almost-periodic solids there appear new types of conductivity, e.g. the Frölich conductivity.

Further, we consider the finite-gap potentials that form a subset in the set of all one-dimensional almost-periodic potentials. These potentials are singled out of other almost-periodic potentials by the following spectral property: the spectrum of the Schrödinger operator with finite-gap potential is double absolutely continuous and consists of a finite number of bands separated by a finite number of gaps. A reader can find the basic information on finite-gap potentials in [8—10].

3. Finite-gap Potentials

The almost-periodic function $u(x)$ is called a finite-gap potential if the spectrum of the Schrödinger operator $L(u) = -\partial_x^2 + u(x)$ is a union of the finite set of segments of a Lebesgue (double absolutely continuous) spectrum $[E_1, E_2] \cup [E_3, E_4] \cup \cdots \cup [E_{2g_1}, \infty]$, where boundaries of the bands supposed to be real and ordered as $E_1 < E_2 \ldots, < E_{2g+1} < +\infty$.

Starting directly from this definition, we can derive an explicit expression and the basic properties of a finite-gap potential [11].

3.1. Number of states and eigenfunctions for a finite-gap potential

Finite-gap potentials are described adequately in the language of hyperelliptic Riemann surfaces. With this aim, let us fix the Riemann surface X of genus g by the equation

$$\mu^2 = R_{2g+1}(\lambda), \quad R_{2g+1}(\lambda) = 4\prod_{k=1}^{2g+1}(\lambda - E_k), \tag{2}$$

and denote the coordinate of the Riemann surface as $P = (\lambda, \mu)$ and the coordinates of branch points as $(E_k, 0)$, $k = 1, \ldots, 2g+1$.

The Weyl function of a finite-gap potential $u(x)$ is defined on the Riemann surface X of a hyperelliptic curve by the formula

$$w(x,P) = \frac{1}{2}\left(\frac{\mu}{S(x,P)} + \imath\frac{\partial_x S(x,P)}{S(x,P)}\right), \tag{3}$$

where

$$S(x,\lambda) = \prod_{k=1}^{g}(\lambda - \lambda_k(x)), \tag{4}$$

and $(\lambda_k(x), \mu_k(x))$, $k = 1, \ldots, g$, is a set of distinct points of the curve X which depends on the variable x.

The quasi-momentum is defined by the expression

$$k(P) = \langle w(P,x)\rangle = \left\langle \frac{\mu}{2S(x,P)}\right\rangle =$$

$$= \int_{(\infty,\infty)}^{P} \frac{\langle 2S(x,P)\rangle}{\mu}\mathrm{d}\lambda, \tag{5}$$

where

$$\langle\, f(x)\rangle = \lim_{L\to\infty}\frac{1}{L}\int_{-L/2}^{L/2} f(x)\mathrm{d}x.$$

The number of states and the quasi-momentum for a finite-gap potential are connected in such a way:

$$N(E) = \frac{1}{\pi}k(E) = \frac{1}{\pi}\left\langle \frac{\sqrt{R_{2g+1}(E)}}{S(x,E)}\right\rangle =$$

$$= \frac{1}{\pi}\int^{E}\left\langle \frac{S(x,E)}{\sqrt{R_{2g+1}(E)}}\right\rangle \mathrm{d}E. \tag{6}$$

The Bloch eigenfunction of the g-gap potential is of the form

$$\psi(x,P) = \sqrt{\frac{S(x,P)}{\langle S(x,P)\rangle}}\exp\left\{\frac{\imath\mu}{2}\int_{x_0}^{x}\frac{\mathrm{d}y}{S(y,P)}\mathrm{d}y\right\}. \tag{7}$$

Here, we assume that the eigenfunction is normalized by the condition

$$\langle|\psi(x,P)|^2\rangle = 1. \tag{8}$$

We now express the basic notions of finite-gap potentials in terms of the sigma-functions with aim to do our further calculations easier.

3.2. σ-functional description of a g-gap potential, number of states, and Bloch eigenfunctions

The g-dimensional σ-function is defined by the formula [12]

$$\sigma(\boldsymbol{h}) = \sqrt{\frac{\pi^g}{\det(2\omega)}}\sqrt[4]{\prod_{1\le i<j\le 2g+1}(E_i - E_j)}\times$$

$$\times\theta((2\omega)^{-1}\boldsymbol{h}|\tau)\exp(\boldsymbol{h}^T\eta(2\omega)^{-1}\boldsymbol{h}|\tau). \tag{9}$$

Here,

$$\boldsymbol{h} = \sum_{k=1}^{g}\int_{\infty}^{\lambda_k}\mathrm{d}u_k - \boldsymbol{K}$$

is the vector of canonical holomorphic differentials, $(\lambda_j, \mu_j), j = 1, \ldots, g$, is a non-special divisor, $\boldsymbol{K}$ is a vector of the Riemann constants, ω and ω' are the $g\times g$ matrices of $a-$ and $b-$periods of canonical holomorphic differentials [12], respectively,

$$\omega = (\omega_{i,k}) = \left(\frac{1}{2}\oint_{\mathfrak{a}_k}\mathrm{d}h_i\right), \quad \omega' = (\omega'_{i,k}) = \left(\frac{1}{2}\oint_{\mathfrak{b}_k}\mathrm{d}h_i\right),$$

$\tau = \omega^{-1}\omega'$ is a matrix in the Siegel upper half-space $\mathcal{S}_g = \{\tau|\tau^T = \tau,\ \mathrm{Im}\tau > 0\ \}$, and $\theta(\boldsymbol{z};\tau)$ is a canonical $g-$dimensional theta-function,

$$\theta(\boldsymbol{z};\tau) = \sum_{\boldsymbol{m}\in\mathbb{Z}^g}\exp\left\{\imath\pi\boldsymbol{m}^T\tau\boldsymbol{m} + 2\imath\pi\boldsymbol{z}^T\boldsymbol{m}\right\}. \tag{10}$$

The σ-function is invariant with respect to the action of certain subgroups of the symplectic group. It also has the following transformation property with respect to the argument shift by the period,

$$\sigma(\boldsymbol{h} + 2\omega\boldsymbol{n} + 2\omega'\boldsymbol{m}) =$$

$$= \sigma(\boldsymbol{h})\exp\left\{(2\eta\boldsymbol{n}+2\eta'\boldsymbol{m})^T(\boldsymbol{h}+\omega\boldsymbol{n}+\omega'\boldsymbol{m}\ )\ \right\},$$

where $\boldsymbol{n},\boldsymbol{m}$ are integer g-vectors and η and η' are the $g\times g$ matrices of $a-$ and $b-$periods of canonical meromorphic differentials $\boldsymbol{r}=(r_1,\dots,r_g)$ [12], respectively,

$$\eta=(\eta_{i,k})=\left(-\frac{1}{2}\oint_{\mathfrak{a}_k}\mathrm{d}r_i\right),\quad \eta'=(\eta'_{i,k})=\left(\frac{1}{2}\oint_{\mathfrak{b}_k}\mathrm{d}r_i\right).$$

Logarithmic derivatives of the σ-function are the g-dimensional ζ and $\wp$-functions,

$$\zeta_i(\boldsymbol{h})=\frac{\partial}{\partial u_i}\log\sigma(\boldsymbol{h}),\quad i=1\dots,g,$$

$$\wp_{i,j}(\boldsymbol{h})=-\frac{\partial^2}{\partial u_i\partial u_j}\log\sigma(\boldsymbol{h}),\quad i,j=1,\dots,g,$$

$$\wp_{i,j,k}(\boldsymbol{h})=-\frac{\partial^3}{\partial u_i\partial u_j\partial u_k}\log\sigma(\boldsymbol{h}),\quad i,j,k=1,\dots,g,\text{etc.}$$

These functions have the periodicity properties

$$\zeta_k(\boldsymbol{u}+2\omega\boldsymbol{n}+2\omega'\boldsymbol{m})=\zeta_k(\boldsymbol{u})+2\eta\boldsymbol{n}+2\eta'\boldsymbol{m},$$

$$k=1,\dots,g,$$

$$\wp_{\mathcal{I}}(\boldsymbol{u}+2\omega\boldsymbol{n}+2\omega'\boldsymbol{m})=\wp_{\mathcal{I}}(\boldsymbol{u}),$$

where $\boldsymbol{n},\boldsymbol{m}\in\mathbb{Z}^g$ are two arbitrary integer vectors and $\mathcal{I}$ is an arbitrary set of two, three, etc. indices.

In terms of g-dimensional hyperelliptic σ-functions, the smooth and real g-gap potential $u(x)$ and the Bloch eigenfunction $\psi(x,P)$ are given by the formulae

$$u(x)=\wp_{gg}(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega}), \tag{11}$$

$$\psi(x,P)=C(P)\frac{\sigma\left(\int_\infty^P\mathrm{d}\boldsymbol{h}-\imath x\boldsymbol{e}_g+\boldsymbol{\Omega}\right)}{\sigma_2\left(\int_\infty^P\mathrm{d}\boldsymbol{h}\right)\sigma(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega})}\times$$

$$\times\exp\left(\imath x\int\limits_{(E_{2g+1},0)}^{P}\mathrm{d}r_g-\boldsymbol{\Omega}^T\int\limits_{E_{2g+1}}^{P}\mathrm{d}\boldsymbol{r}\right), \tag{12}$$

where

$$\boldsymbol{e}_g=(0,\dots,0,1)^T,\quad \sigma(\boldsymbol{v})=\sigma_g(\boldsymbol{v})=\dots=\sigma_{g-2}(\boldsymbol{v})=0,$$

$$\boldsymbol{v}=\left(\int_\infty^P\mathrm{d}h_1,\dots,\int\limits_\infty^P\mathrm{d}h_g\right)^T,$$

$\boldsymbol{\Omega}=(\Omega_1,\dots,\Omega_g)^T$ are not purely imaginary even half-period supported by g branch points, and $\mathrm{d}r_1,\dots,\mathrm{d}r_g$ are canonical meromorphic differentials.

The Weyl function $w(x,P)$ and wave number $k(P)$ in terms of σ-functions look as follows:

$$w(x,P)=\zeta_g\left(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega}+\int\limits_{E_{2g+1}}^{P}\mathrm{d}\boldsymbol{h}\right)-$$

$$-\zeta_g(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega})-\int\limits_{E_{2g+1}}^{P}\mathrm{d}r_g,$$

$$k(P)=\left\langle\zeta_g\left(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega}+\int\limits_{\infty}^{P}\mathrm{d}\boldsymbol{h}\right)-\right.$$

$$\left.-\zeta_g(\imath x\boldsymbol{e}_g-\boldsymbol{\Omega})-\int\limits_{E_{2g+1}}^{P}\mathrm{d}r_g\right\rangle.$$

4. Averages for Periodic and Almost-periodic Finite-gap Potentials

The averaging over a finite-gap potential is different for two classes of finite-gap potentials - periodic and almost-periodic ones. They correspond to periodic and ergodic averages, respectively.

4.1. Periodic and ergodic finite-gap potential

We call the $g-$dimensional vector

$$\boldsymbol{U}=(U_1,\dots,U_g)^T=(2\omega')^{-1}\boldsymbol{e}_g \tag{13}$$

as a winding vector of the finite-gap potential (11). A finite-gap potential is called periodic if there exists an integer vector $\boldsymbol{n}\in\mathbb{Z}^g$ and a real number $U\in\mathbb{R}$, $U\neq 0$, such that

$$\boldsymbol{U}=\boldsymbol{n}U. \tag{14}$$

Otherwise, a finite-gap potential is called properly almost-periodic (or ergodic).

In generic case, a finite-gap potential is obviously ergodic, it is periodic only under the special conditions presented above.

According to the above definition, a finite gap-potential is periodic if, for a certain vector $\boldsymbol{n} \in \mathbb{Z}^g$ and a real number $U \neq 0$, the period matrix $2\omega'$ of a curve X satisfies the equation

$$\omega' \boldsymbol{n} = \frac{1}{2U} \boldsymbol{e}_g \tag{15}$$

which represents g transcendental conditions on the moduli of the curve.

One can easily see that, under this condition, the functions $g_{kl}(x) = \wp_{kl}\left(\imath x \boldsymbol{e}_g - \boldsymbol{\Omega}\right)$ are periodic in x with the period $\imath/U$. Indeed,

$$\wp_{kl}\left(\imath\left(x + \frac{\imath}{U}\right)\boldsymbol{e}_g - \boldsymbol{\Omega}\right) =$$

$$= \wp_{kl}\left(\imath x \boldsymbol{e}_g - \boldsymbol{\Omega} - 2\omega' \boldsymbol{n}\right) = \wp_{kl}\left(\imath x \boldsymbol{e}_g - \boldsymbol{\Omega}\right).$$

The conditions of periodicity (15) are weaker than the conditions of double periodicity in x of finite-gap potentials. The last conditions are formulated in terms of the period matrix of the curve τ as follows [13].

A finite-gap potential $u(x)$ is an elliptic function of x if and only if there exists such a homology basis that the period matrix τ has the form

$$\tau = \begin{pmatrix} \tau_{11} & k/N & 0 & \dots & 0 \\ k/N & * & * & * & * \\ 0 & * & * & * & * \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & * & * & * & * \end{pmatrix} \tag{16}$$

and, in this basis, the winding vector is of the form

$$\boldsymbol{U} = (*, 0, \dots, 0)^T. \tag{17}$$

Conditions (16), (17) represent $2g-2$ equations and, therefore, the associated double periodic potentials represent a very particular subset of periodic potentials. These particular potentials allow an explicit analytic description, and we use this circumstance in what follows.

Conditions (16), (17) are studied in the reduction theory of Abelian functions to elliptic ones which goes back to Jacobi, Weierstrass and Poincaré. The modern exposition and applications to integrable system are given, in particular, in [14, 15].

4.2. Averages in periodic and ergodic cases

Our discussion and the calculation of averages in the periodic and ergodic cases are similar to those in [16]. We should remark that calculations of ergodic averages for almost-periodic finite-gap objects were fulfilled for the first time in [17].

The average of any object of our theory is sensible to the commensurability or inconmmensurability of frequencies (components of the winding vector $\boldsymbol{U}$). Hence in what follows, we specify the average of any quantity in the periodic case with the super(or sub)script (p), and the same quantity in the ergodic case with the super(or sub)script (e). For example, we provide $\langle S(x,\lambda)\rangle$ with subscripts, $\langle S(x,\lambda)\rangle^{(p)}$ and $\langle S(x,\lambda)\rangle^{(e)}$.

Ergodic case. Let the components of the winding vector $\boldsymbol{U}$ be all incommensurable. Then the average $\langle S(x,\lambda)\rangle^{(e)}$ is ergodic and is

$$\langle S(x,\lambda)\rangle^{(e)} = \lambda^g + \sum_{j=1}^{g} \lambda^{j-1} s_j^{(e)} \tag{18}$$

where

$$s_j^{(e)} = \frac{1}{\det 2\omega'} \det \begin{pmatrix} \omega'_{1,1} & \dots & \omega'_{1,g} \\ \vdots & \dots & \vdots \\ \omega'_{j-1,1} & \dots & \omega'_{j-1,g} \\ \eta'_{g,1} & \dots & \eta'_{g,g} \\ \omega'_{j+1,1} & \dots & \omega'_{j+1,g} \\ \vdots & \dots & \vdots \\ \omega'_{g,1} & \dots & \omega'_{g,g} \end{pmatrix},$$

$j = 1, \dots, g$.

In particular, at $g = 1$,

$$\langle S(x,\lambda)\rangle^{(e)} = \lambda + \frac{\eta'}{\omega'},$$

and, at $g = 2$,

$$\langle S(x,\lambda)\rangle^{(e)} = \lambda^2 + \lambda \frac{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \eta'_{21} & \eta'_{22} \end{pmatrix}}{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \omega'_{21} & \omega'_{22} \end{pmatrix}} -$$

$$- \frac{\det \begin{pmatrix} \omega'_{21} & \omega'_{22} \\ \eta'_{21} & \eta'_{22} \end{pmatrix}}{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \omega'_{21} & \omega'_{22} \end{pmatrix}}.$$

Periodic case. Let the components of the winding vector $\boldsymbol{U}$ be all commensurable. Then the average $\langle S(x,\lambda)\rangle^{(p)}$ is periodic and is

$$\langle S(x,\lambda)\rangle^{(p)} = \lambda^g + \sum_{j=1}^{g} \lambda^{j-1} s_j^{(p)}, \tag{19}$$

where

$$s_j^{(p)} = \frac{1}{\det 2\omega'} \det \begin{pmatrix} \omega'_{1,1} & \dots & \omega'_{1,g} \\ \vdots & \dots & \vdots \\ \omega'_{g-1,1} & \dots & \omega'_{g-1,g} \\ \eta'_{j,1} & \dots & \eta'_{j,g} \end{pmatrix},$$

$$j = 1, \dots, g. \tag{20}$$

In particular, at $g = 1$,

$$\langle S(x,\lambda)\rangle^{(p)} = \lambda + \frac{\eta'}{\omega'},$$

and, at $g = 2$,

$$\langle S(x,\lambda)\rangle^{(p)} = \lambda^2 + \lambda \frac{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \eta'_{21} & \eta'_{22} \end{pmatrix}}{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \omega'_{21} & \omega'_{22} \end{pmatrix}} +$$

$$+ \frac{\det \begin{pmatrix} \omega'_{21} & \omega'_{22} \\ \eta'_{11} & \eta'_{12} \end{pmatrix}}{\det \begin{pmatrix} \omega'_{11} & \omega'_{12} \\ \omega'_{21} & \omega'_{22} \end{pmatrix}}.$$

We see that averages in the ergodic and periodic cases coincide for elliptic curves. But, starting from genera 2, the periodic and ergodic averages are different.

5. Free Energy and Commensurability Energy of a Solid with Finite-gap Structure

Let us consider the free energy F of a solid which consists of the deformed lattice and electrons. In this case, we obviously have

$$F = F_{\text{elect}} + F_{\text{latt}}.$$

If the electrons do not interact with one another and move in a potential $u(x)$ created by the deformed lattice, then

$$F_{\text{elect}} = \mu N - \int \mathrm{d}E N(u(\cdot), E) f(E),$$

where μ is the chemical potential, N is the density of electrons, $N(u(\cdot), E)$ is the number of electrons per unit length with energy less than E in the potential $u(x)$, and $f(E)$ is the Fermi—Dirac distribution for temperature T,

$$f(E) = [\exp(E-\mu)/T + 1]^{-1}.$$

5.1. Free energy of a solid with finite-gap structure

If the lattice is deformed in such a way that it creates a g-gap potential $u(x)$ for electrons, then

$$F_{\text{latt}} = \sum_{i=-1}^{g} c_i I_i.$$

Here, $c_i, i = -1, 0, 1, \dots, g$, are some constants and

$$I_i = \langle\, \chi_i \rangle = \lim_{L\to\infty} \frac{1}{L} \int_{-L/2}^{L/2} \chi_i(x)\mathrm{d}x, \quad i = -1, 0, 1, \dots,$$

are the Novikov—Bogoyavlenski integrals [8]. For small indices i, these integrals looks as follows:

$$I_{-1} = \langle u \rangle, \quad I_0 = \langle u^2 \rangle, \quad I_1 = 2\langle u^3 \rangle + \langle (u')^2 \rangle,$$

$$I_2 = 5\langle u^4 \rangle + 10\langle u(u')^2 \rangle + \langle (u'')^2, \rangle \quad \text{etc.}$$

Let us also take in account that the density of states of electrons in a g-gap potential is of the form

$$N(u(\cdot), E) = \frac{1}{\pi} \int^{E} \frac{\langle S(x,E)\rangle}{\sqrt{R_{2g+1}(E)}},$$

where

$$\langle S(x,E)\rangle = \left\langle \prod_{k=1}^{g} (E - \lambda_k(x)) \right\rangle,$$

and the symmetrized products of $\lambda_k(x), k = 1, \dots, g$, are polynomials of the potential $u(x)$ and its derivatives due to the so-called trace formulae,

$$\sum_j \lambda_j(x) = -\frac{1}{4}\frac{\delta I_0}{\delta u(x)} + \frac{1}{2}\sum_i E_i,$$

$$\sum_{j<k} \lambda_j(x)\lambda_k(x) = \frac{1}{16}\frac{\delta I_1}{\delta u(x)} -$$

$$-\frac{1}{8}\frac{\delta I_0}{\delta u(x)}\sum_i E_i - \sum_i E_i^2 + \frac{1}{8}\left(\sum_i E_i\right)^2, \quad \text{etc.}$$

With all these assumptions, the free energy of such a solid looks as

$$F = \mu N - \int \mathrm{d}E f(E) N(u(\cdot), E) + \sum_{i=-1}^{g} c_i I_i = \mu N -$$

$$- \int \mathrm{d}E f(E) \frac{1}{\pi} \int^E \mathrm{d}E \frac{\langle S(x,E)\rangle}{\sqrt{R_{2g+1}(E)}} + \sum_{i=-1}^{g} c_i \langle \chi_i \rangle, \qquad (21)$$

i.e. the free energy is the average of some polynomial of the potential $u(x)$ and its derivatives.

We would like to mention here that, according to our assumption, a solution of the variation equation $\delta F_{\mathrm{latt}}/\delta u(x) = 0$ is a g-gap potential, but a solution of the variation equation $\delta F/\delta u(x) = 0$ may be a $(g+1)$-gap potential, i.e. the equilibrium g-gap lattice potential can transform under the influence of electrons to an equilibrium $(g+1)$-gap potential [18].

5.2. The commensurability energy

Thus, according to the above discussion, the commensurability energy of a solid is

$$\Delta F = F^{(e)} - F^{(p)} = \sum_{i=-1}^{g} c_i [\langle \chi_i \rangle^{(e)} - \langle \chi_i \rangle^{(p)}] -$$

$$- \int \mathrm{d}E f(E) \frac{1}{\pi} \int^E \mathrm{d}E \frac{\langle S(x,E)\rangle^{(e)} - \langle S(x,E)\rangle^{(p)}}{\sqrt{R_{2g+1}(E)}}. \qquad (22)$$

Let us consider some examples.

One-gap potential. For a one-gap potential, the commensurability energy is

$$\Delta F = F^{(e)} - F^{(p)} = c_0 [\langle \chi_0 \rangle^{(e)} -$$

$$- \langle \chi_0 \rangle^{(p)}] + c_{-1} [\langle \chi_{-1} \rangle^{(e)} \langle \chi_{-1} \rangle^{(p)}] +$$

$$+ \int \mathrm{d}E f(E) \frac{1}{\pi} \int^E \mathrm{d}E \frac{\langle \lambda_1(x) \rangle^{(e)} - \langle \lambda_1(x) \rangle^{(p)}}{\sqrt{R_3(E)}}.$$

Since the averages for a one-gap potential in the ergodic and periodic cases coincide, the commensurability energy

$$\Delta F = 0.$$

Two-gap potential. For a two-gap potential, the commensurability energy is

$$\Delta F = F^{(e)} - F^{(p)} = c_1 [\langle \chi_1 \rangle^{(e)} - \langle \chi_1 \rangle^{(p)}] +$$

$$+ c_0 [\langle \chi_0 \rangle^{(e)} - \langle \chi_0 \rangle^{(p)}] + c_{-1} [\langle \chi_{-1} \rangle^{(e)} \langle \chi_{-1} \rangle^{(p)}] +$$

$$+ \int \mathrm{d}E f(E) \times$$

$$\times \frac{1}{\pi} \int^E \mathrm{d}E E \frac{\langle \lambda_1(x) + \lambda_2(x) \rangle^{(e)} - \langle \lambda_1(x) + \lambda_2(x) \rangle^{(p)}}{\sqrt{R_5(E)}} -$$

$$- \int \mathrm{d}E f(E) \frac{1}{\pi} \int^E \mathrm{d}E \frac{\langle \lambda_1(x)\lambda_2(x) \rangle^{(e)} - \langle \lambda_1(x)\lambda_2(x) \rangle^{(p)}}{\sqrt{R_5(E)}}.$$

6. Conclusion

Thus, we have calculated the commensurability energy of a solid with finite-gap structure by means of a consistent and rigorous procedure and have obtained the explicit formulae for it. In particular, we have shown that the commensurability energy for a one-gap structure is equal to zero. But, starting from two-gap structures, the commensurability energy does not vanish in general case.

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ЕНЕРГІЯ СУМІРНОСТІ ТВЕРДИХ ТІЛ

Є.Д. Білоколос

Р е з ю м е

Різниця енергій між сумірними (періодичними) та несумірними (майже періодичними) структурами твердого тіла (так звана енергія сумірності) розрахована для одновимірної моделі твердого тіла із скінченно-зонним потенціалом.

ЕНЕРГИЯ СОИЗМЕРИМОСТИ ТВЕРДЫХ ТЕЛ

Е.Д. Белоколос

Р е з ю м е

Разница енергий между соизмеримыми (периодическими) и несоизмеримыми (почти периодическими) структурами твердого тела (так называемая енергия соизмеримости) расчитана для одномерной модели твердого тела с конечно-зонным потенциалом.