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Spectra of the Schrödinger Operators with Finite-Gap Potentials and Integrable Systems

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The report presents results of studies of spectral properties of the Schrödinger operators with finite-gap potentials along with their applications to problems of physics of solids. As an example of these applications we consider the Peierls problem.

1 Introduction

Recently a deep connection of spectral properties of the Schrödinger operators with periodic finite- and infinite-gap potentials was discovered, and also their relations with the theory of integrable systems were established. Last property allows to describe effectively the spectrum, eigenvalues, eigenfunctions and also matrix elements of any observable analytically. Application of these results to physics of solids appears to be very successful for explanation and quantitative description of many phenomena and properties of solids. Construction of the separable many-dimensional generalization of the one-dimensional finite-gap potentials is very interesting since it which allows to solve a number of 3-dimensional practical problems of solid state physics.

2 The Schrödinger operator with finite-gap potential

2.1 The one-gap potential

Let us consider the Schrödinger equation with the Weierstrass function $\wp(z)$ as the potential,

$$-\partial_x^2\psi(x) + u(x)\psi(x) = \epsilon\psi(x), \qquad u(x) = -2\wp(\imath x + \omega), \quad x \in \mathbb{R}.$$

We use here and further the traditional notations of the theory of elliptic functions. An average value of the potential is

$$\langle u(x)\rangle = -2\langle\wp(\imath x + \omega)\rangle = 2\eta'/\omega'.$$

Here and further

$$\langle g\rangle = \lim_{l\to\infty} L^{-1}\int_0^L g(x)\mathrm{d}x.$$

The following statements are simple consequences of the formulae from the elliptic functions theory.

The potential $u(x) = -2\wp(\imath x + \omega)$ has a real period $T = -\imath 2\omega'$ and an imaginary period $T' = \imath 2\omega$. The potential $u(x)$ is a linear superposition of solitons,

$$u(x) = 2\frac{\eta}{\omega} - 2\left(\frac{\pi}{2\omega}\right)^2 \sum_{n=-\infty}^{+\infty} \cosh^{-2}\left[\frac{\imath\pi}{2\omega}(\imath x - n2\omega')\right].$$

We can present the eigenfunction of the Schrödinger operator with the one-gap potential in terms of the σ-functions

$$\psi_{\pm}(x) = \frac{\sigma(\imath x + \omega \pm z)}{\sigma(\imath x + \omega)\sigma(z)} e^{\mp \imath x \zeta(z)},$$

or in terms of the potential $u(x)$, or $\wp$-function,

$$\psi(x,\varepsilon) = [\langle \chi^{-1}(x,\varepsilon)\rangle \chi(x,\varepsilon)]^{-1/2} \exp\left(\imath \int^x \mathrm{d}x\, \chi(x,\varepsilon)\right),$$
$$\chi(x,\varepsilon) = [P(\varepsilon)]^{1/2}\big(\varepsilon - \gamma(x)\big)^{-1}, \qquad P(\varepsilon) = (\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3),$$
$$\gamma(x) = (1/2)\big(\varepsilon_1+\varepsilon_2+\varepsilon_3 - u(x)\big).$$

In the last form the wave function is normalized by a condition $\langle |\psi|^2\rangle = 1$.

The wave function is defined on the two sheets of a Riemann surface given by the equation $\mu^2 = P(\varepsilon) = (\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)$.

The spectrum Σ of the Schrödinger operator with the one-gap potential is

$$\epsilon = \wp(z),$$
$$z = \omega' + t\omega, \quad 0 \le t \le 1, \quad \text{or}$$
$$z = \omega + t\omega', \quad 0 \le t \le 1.$$

Therefore the spectrum Σ has one finite energy band $e_3 \le \epsilon \le e_2$ when $z = \omega' + t\omega$, $0 \le t \le 1$, the energy gap $e_2 \le \epsilon \le e_1$ when $z = \omega + t\omega'$, $0 \le t \le 1$, and one infinite energy band $e_1 \le \epsilon < +\infty$ when $z = \omega + t\omega$, $0 \le t \le 1$.

The eigenfunctions $\psi_{\pm}(x)$ satisfy the Floquet equality $\psi(x+T) = e^{\imath kT}\psi(x)$ and have the Bloch form $\psi(x) = A(x)e^{\imath kx}$ where $A(x)$ is the periodic amplitude, $A(x+T) = A(x)$, and k is the wave vector

$$k = \zeta(z) - z(\eta'/\omega'), \quad z = \omega' + t\omega, \quad 0 \le t \le 1;$$
$$k = -[\zeta(z) - z(\eta'/\omega')], \quad z = \omega + t\omega, \quad 0 \le t \le 1.$$

Due to the oscillation theorem the density of states $n = k/\pi$.

A number of states over a unit of length with the energy less than ε is

$$n(u(\cdot),\varepsilon) = \frac{1}{\pi}\langle \chi(x,\varepsilon)\rangle = \frac{1}{\pi}\sqrt{(\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)}\langle(\varepsilon-\gamma(x))^{-1}\rangle.$$

Here ε_1, ε_2, ε_3, $\varepsilon_1 \le \varepsilon_2 \le \varepsilon_3$ are the boundaries of the spectrum.

This quantity satisfies important relations:

$$\frac{\mathrm{d}n}{\mathrm{d}\varepsilon}(u(\cdot),E) = \frac{1}{2\pi}\langle \chi^{-1}(x,\varepsilon)\rangle, \qquad \frac{\delta n}{\delta u(x)}(u(\cdot),\varepsilon) = -\frac{1}{2\pi}\chi^{-1}(x,\varepsilon).$$

Here $(\delta n/\delta u(x))(u(\cdot),\varepsilon)$ is a variational derivative of the number of states n with respect to such variations of the potential which do not change its periods.

3 The finite-gap potentials

3.1 One-dimensional finite-gap potentials

A one-gap potential $u(z) = 2\wp(z)$ is a special case of the Lame potentials

$$u(z) = n(n+1)\wp(z), \qquad n \in \mathbb{N}.$$

The Schrödinger operator with the Lamé potential has the n-gap spectrum and the following two linearly independent eigenfunctions:

$$\Psi_{\pm}(x;z)=\prod_{r=1}^{n}\left\{\frac{\sigma(a_r+x)}{\sigma(a_r)\sigma(x)}\right\}\exp\left\{\pm x\sum_{r=1}^{n}\zeta(a_r)\right\}.$$

The Lame potentials present a particular case of the Darboux potentials which are linear superpositions of the Weierstrass functions with shifts of the following form

$$u(x)=n_0(n_0+1)\wp(x)+\sum_{i=1}^{3}n_i(n_i+1)\wp(x+\omega_i),$$

where ω_i, $i=1,2,3$ are half-periods. If $n_i=0$, $i=1,2,3$ we have the Lame potential.

The Darboux potential is characterized completely by the four integers $n_0,n_1,n_2,n_3\in\mathbb{Z}_+$. If the Darboux potential is associated with the hyperelliptic curve $w^2=P_{2g+1}(E)$ then its genus is equal to g. This curve covers N-sheetedly an elliptic curve and

$$N=\frac{1}{2}\left\{n_0(n_0+1)+\sum_{i=1}^{3}n_i(n_i+1)\right\}.$$

A list of some Darboux potentials [15].

- $\mathbf{0},\mathbf{0},\mathbf{0},\mathbf{0}$, $g=0$, $N=0$.
  $u(x)=0$; $w^2=\mu$.
- $\mathbf{1},\mathbf{0},\mathbf{0},\mathbf{0}$, $g=1$, $N=1$.
  $u(x)=2\wp(x)$; $w^2=(\mu-e_1)(\mu-e_2)(\mu-e_3)$.
- $\mathbf{1},\mathbf{1},\mathbf{0},\mathbf{0}$, $g=1$, $N=2$.
  $u(x)=-2e_1+2\wp(x)+2\wp(x+\omega_1)$;
  $w^2=(\mu+2e_1)(\mu^2-2e_1\mu-11e_1^2+g_2)$.
- $\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{0}$, $g=2$, $N=3$.
  $u(x)=2\wp(x)+2\wp(x+\omega_1)+2\wp(x+\omega_2)$;
  $w^2=(\mu+3e_1)(\mu+3e_2)(\mu+3e_3)(\mu^2-3g_2)$.
- $\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{1}$, $g=1$, $N=4$.
  $u(x)=2\wp(x)+2\wp(x+\omega_1)+2\wp(x+\omega_2)+2\wp(x+\omega_3)$;
  $w^2=(\mu-4e_1)(\mu-4e_2)(\mu-4e_3)$.

The periodic elliptic finite-gap potentials are a very special case of the general finite-gap potentials which are described in terms of the hyperelliptic functions and in generic situation are the quasi-periodic functions.

Definition 1. The almost-periodic function $u(x)$ is called a finite-band 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.

Starting directly from this definition we can derive an explicit expression of a finite-band potential.

Theorem 1 ([13]). *The potential $u(x)$ of the Schrödinger operator $L(u)=-\partial_x^2+u(x)$ with the g-gap Lebesgue spectrum*

$$\Sigma=[E_1,E_2]\cup\cdots\cup[E_{2g+1},\infty)$$

has the form

$$u(x) = -2\partial_x^2 \ln\theta\left(\imath\vec{U}x - \vec{A}(D) + \vec{K}, B\right).$$

Here B is the matrix of the periods of normalized holomorphic differentials $\vec{\omega}$ on the hyperelliptic Riemann surface X, defined by the equation

$$\mu^2 = \prod_{i=1}^{2g+1}(\lambda - E_i),$$

$\vec{K}$ is the vector of Riemann constants, $\vec{U}$ is the vector of the periods of the normalized Abelian differential Ω of the second kind, which at infinity has a second-order pole with zero residue, D is a non-special divisor, $\vec{A}(D) = \int_\infty^P \vec{\omega}$ is an Abelian mapping.

By means of the Weierstrass–Poincaré theory of the Abelian function reduction we can point out conditions when these general finite-gap potentials become elliptic and fulfill this reduction effectively [7, 8].

3.2 Separable many-dimensional finite-gap potential

In the framework of the complex analysis there are no many-dimensional generalizations of the finite-gap potentials besides only trivial (i.e. separable) many-dimensional finite-gap potentials [11].

Let us consider a d-dimensional Schrödinger operator

$$H = -\Delta + U(x_1, x_2, \ldots, x_d) \tag{1}$$

with a periodic separable finite-gap potential of the form

$$U(x_1, x_2, \ldots, x_d) = \sum_{i=1}^{d} u(x_i), \tag{2}$$

where $u(x_i)$, $i = 1, 2, \ldots, d$ are some 1-dimensional finite-gap potentials (e.g. the Lamé potentials, the Darboux potentials etc.). In spite of triviality of this Hamiltonian it appears to be successful in applications. As an example we apply it to the quantum theory of solids with $d = 3$.

A limit case $U(x_1, x_2, x_3) \to 0$ of the operator (1) has been used with success in theory of solids in order to describe the electron energy spectra and classify all possible Fermi surfaces of metals [12]. Harrison's method is in fact a theory of almost free electrons when the potential is considered as a perturbation. Usage of the separable finite-gap potentials (2) is an essential step ahead with respect to Harrison's method since it allows consider limit cases of the free and strongly bound electrons in frame of the same model.

We have used the separable finite-gap potentials to describe many phenomena and properties of solids: the electron energy spectra of solids and Fermi surfaces of metals, the scattering and absorption of electromagnetic and other waves by finite-gap solids, the electron-phonon interaction, the Peierls transition and Fröhlich conductivity, the classification of the quasi-one-dimensional conductors, the oscillations in solids due to isospectral deformations of finite-gap potentials etc. Results of these studies are presented in recent publications [1, 2, 6].

4 The Peierls problem

The Peierls problem is to find eigenstates and eigenvalues of the electron-phonon Hamiltonian, defined on a segment $[0, L]$,

$$H = \sum_{k,\sigma} \epsilon_k a^+_{k,\sigma} a_{k,\sigma} + \sum_q \omega_q b^+_q b_q + L^{-1/2} \sum_q (\lambda_q L_q b^+_q + \lambda^*_q L^+_q b_q),$$
$$L_q = \sum_{k,\sigma} a^+_{k,\sigma} a_{k+q,\sigma}.$$

Here $a^+_{k,\sigma}$, $a_{k,\sigma}$ are electron operators; b^+_q, b_q are phonon operators; L^+_q, L_q are operators for charge density waves; ϵ_k, ω_q are the energies of electrons and phonons appropriately, λ_q is the electron-phonon interaction constant.

The exact solution of the Peierls problem was found recently [3, 4, 5].

When the mean field approximation is valid then we have in thermodynamic limit the condensation of phonons and charge density waves,

$$L^{-1/2} b^\#_q = \xi^\#_q + (L^{-1/2} b^\#_q - \xi^\#_q), \qquad \xi^\#_q = L^{-1/2} \langle b^\#_q \rangle,$$
$$L^{-1} L^\#_q = \eta^\#_q + (L^{-1} L^\#_q - \eta^\#_q), \qquad \eta^\#_q = L^{-1} \langle L^\#_q \rangle.$$

Here $\langle F \rangle$ stands for the statistical average of the operator F and therefore $\xi^\#_q$, $\eta^\#_q$ are statistical averages of the operators $b^\#_q$, $L^\#_q$. The operators $L^{-1/2} b^\#_q - \xi^\#_q$, $L^{-1} L^\#_q - \eta^\#_q$ describe the quantum fluctuations with respect to mean values.

Thus we can represent the Fröhlich Hamiltonian in the following form

$$H = H_A + V = (H_0 + H_e + H_{ph}) + V,$$

where

$$H_0 = -L \sum_q \left(\frac{|\lambda_q|^2 |\eta_q|^2}{\omega_q} + \lambda_q \eta_q \xi^*_q + \lambda^*_q \eta^*_q \xi_q \right),$$
$$H_e = \sum_{k,\sigma} \epsilon_k a^+_{k,\sigma} a_{k,\sigma} + \sum_q (L_q \lambda_q \xi^*_q + L^+_q \lambda^*_q \xi_q),$$
$$H_{ph} = L \sum_q \omega_q \left(\frac{b^+_q}{L^{1/2}} + \frac{\lambda^*_q \eta^*_q}{\omega_q} \right) \left(\frac{b_q}{L^{1/2}} + \frac{\lambda_q \eta_q}{\omega_q} \right),$$
$$V = \sum_q \left[\lambda_q \left(\frac{L_q}{L} - \eta_q \right) \left(\frac{b^+_q}{L^{1/2}} - \xi^*_q \right) + \lambda^*_q \left(\frac{L^+_q}{L} - \eta^*_q \right) \left(\frac{b_q}{L^{1/2}} - \xi_q \right) \right].$$

The electron Hamiltonian H_e describes a motion of the electrons in the classical field, which appears as a result of the condensation of phonons, the phonon Hamiltonian H_{ph} describes quantum fluctuations of phonons with respect to their classical average values and the interaction part of the Hamiltonian V describes the interaction of the quantum fluctuation of phonons and the charge density waves.

Let us assume that the self-consistency condition is satisfied,

$$L^{-1/2} \langle b_q \rangle = \xi_q = -(\lambda_q/\omega_q) \eta_q = -(\lambda_q/\omega_q) L^{-1} \langle L_q \rangle.$$

Under this condition in the thermodynamic limit we can neglect the interaction V and as a result of that the Fröhlich Hamiltonian H appears to be thermodynamically equivalent to the

quadratic approximating Hamiltonian H_A. It means that the densities of the thermodynamic potentials for both Hamiltonians are equal.

We assume further that

$$\epsilon_k = k^2, \qquad \omega_q \sim q, \qquad \lambda_q \sim q^{1/2}.$$

The last two equalities are valid for acoustic phonons. With this assumption we have

$$\omega_q/|\lambda_q|^2 = \kappa,$$

and therefore the self-consistency condition attains the form

$$\eta_q = -\kappa\lambda_q^*\xi_q.$$

Multiplying the self-consistency condition by $\exp(\imath qx)$ and summing up over q we present this condition in the form

$$\sum_\sigma \langle\psi^+(x,\sigma)\psi(x,\sigma)\rangle = -\kappa u(x).$$

Here we have introduced notations

$$\psi(x,\sigma) = L^{-1/2}\sum_{k,\sigma} a_{k,\sigma}\exp(\imath kx), \qquad u(x) = \sum_q \lambda_q\xi_q\exp(\imath qx),$$

where $\psi(x,\sigma)$ is the electron field operator and $u(x)$ is the classical potential, in which the non-interacting electrons move, according to the electron Hamiltonian H_e.

Diagonalizing the Hamiltonian H_e we can present the electron field operator in the form

$$\psi(x,\sigma) = \sum_{E,\sigma} a_{E,\sigma}\phi(x,E).$$

Here eigenfunctions $\phi(x,E)$ are solutions of the Schrödinger equation

$$\partial_x^2\phi(x,E) + (E-u(x))\phi(x,E) = 0,$$

and the operators $a^{\#}_{E,\sigma}$ satisfy the relations

$$[a^+_{E,\sigma}, a_{E',\sigma'}] = \delta_{E,E'}\delta_{\sigma,\sigma'}, \qquad \langle a^+_{E,\sigma}a_{E',\sigma'}\rangle = \delta_{E,E'}\delta_{\sigma,\sigma'}f(E),$$

where $f(E)$ is the Fermi distribution function. Using this form of the electron field operator we can present the self-consistency condition as follows,

$$\sum_{E,\sigma} f(E)|\phi(x,E)|^2 = -\kappa u(x).$$

The function $|\phi(x,E)|^2$ as a product of two solutions of the Schrödinger equation satisfy the equation

$$\left(\partial_x^3 - 4u(x)\partial_x - 2\partial_x u(x)\right)|\phi(x,E)|^2 = -4E|\phi(x,E)|^2.$$

Let us multiply this equation by the Fermi–Dirac function $f(E)$, sum it up over E and take in account the self-consistency condition. Then we get

$$u_{xxx} - 6uu_x = 4\kappa^{-1}\partial_x\sum_{E,\sigma} Ef(E)|\phi(x,E)|^2.$$

The sum in the r.h.s. of this equation is the energy of electrons and in equilibrium must not depend on a point x (otherwise the electrons will move from one point to another). Therefore

$$u_{xxx} - 6uu_x = 0.$$

Integrating this equation twice we get

$$(u_x)^2 = 2u^3 - 2g_2u - g_3.$$

Since the Weierstrass elliptic function satisfy the equation

$$\left[\wp(z)'\right]^2 = 4\wp^3(z) - g_2\wp(z) - g_3,$$

we can express the potential $u(x)$ in terms of this function [9, 10]

$$u(x) = -2\wp(\imath x + \omega).$$

If we put in the self-consistency condition

$$\sum_{\varepsilon,\sigma} f(\varepsilon)|\phi(x,\varepsilon)|^2 = \kappa u(x)$$

the expression

$$|\phi(x,\varepsilon)|^2 = \left[\langle\chi^{-1}(x,\varepsilon)\rangle\chi(x,\varepsilon)\right]^{-1} = \frac{\varepsilon - \gamma(x)}{\varepsilon - \langle\gamma(x)\rangle},$$

we can present this condition in the form

$$\frac{1}{2\pi}\int_{\varepsilon\in\Sigma} d\varepsilon f(\varepsilon)\frac{\varepsilon - \gamma(x)}{\sqrt{(\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)}} = -\kappa u(x).$$

Equating coefficients at the constant term and $u(x)$ at both sides of the last equality we get two equations

$$\frac{1}{2\pi}\int_{\varepsilon\in\Sigma} d\varepsilon f(\varepsilon)\frac{\varepsilon - (1/2)(\varepsilon_1+\varepsilon_2+\varepsilon_3)}{\sqrt{(\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)}} = 0,$$
$$\frac{1}{4\pi}\int_{\varepsilon\in\Sigma} d\varepsilon f(\varepsilon)\frac{1}{\sqrt{(\varepsilon-\varepsilon_1)(\varepsilon-\varepsilon_2)(\varepsilon-\varepsilon_3)}} = -\kappa.$$

Solving these equations we can define two parameters that characterize the potential $u(x)$, i.e. g_2, g_3, or ω, ω'.

We can solve these equations easily for the absolute zero of temperature when

$$f(\varepsilon) = \theta(\mu - \varepsilon).$$

In such a way we obtain the Peierls equation

$$\omega' = \imath/2\mathcal{N},$$

and the Fröhlich equation

$$\omega = 2\pi\kappa.$$

Here $\mathcal{N}$ is the number of states in the finite energy band.

5 Conclusion

Algebraic finite-gap potentials have deep connections to many areas of mathematics and physics, e.g. to complex analysis, integrable systems etc. They have proved also to be useful in different applications. For example, since we can approximate any smooth periodic potential by the finite-gap one with any desired accuracy [14] we obtain possibility to describe spectral properties of the Schrödinger operator with periodic potential of general form. Although the separable many-dimensional generalizations of the one-dimensional finite-gap are simple they appears also to be effective for solution of a number problems of 3-dimensional physics of solids due to their tight relation to the well known Harrison method. We believe that these potentials will have a lot of interesting applications in future.

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