Micro spectral properties of crystals and their band structure *

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1 Introduction

A multichannel Schrödinger equation with periodic matrix potential is investigated. Such equations arise during the reduction of a multidimensional Schrödinger equation, periodic in one direction, to a set of connected one-dimensional equations. Equations of this type describe the electron spectrum in a solid state, superlattices and low dimensional lattices. Every periodic potential $V(x)$ with the period a can be presented by a sum of infinite number of short range potentials

$$V(x) = \sum_{n \in \mathbf{Z}} v(x - na).$$

The potential $v(x)$ describes the structure of an isolated center. We focus our attention on the relations between the spectral properties of the single scattering center and the band structure of the periodic problem.

The first section is devoted to the finite dimensional matrix Schrödinger equation. Relations between the scattering on a finite crystal and corresponding periodic problem are clarified. It is shown that the bound states corresponding to a single center determine bands of the continuous spectrum

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of the periodic problem and resonances determine spectral gaps in the spectrum. The second section is devoted to the scattering on a one-dimensional chain in the three-dimensional space, which corresponds to the case of an infinite dimensional matrix potential. Exactly solvable model is constructed with the help of the zero range potential method.

2 One dimensional crystal

2.1 Infinite and finite crystals: scattering matrix and band structure

Consider the matrix Schrödinger operator

$$H = -\frac{\partial^2}{\partial x^2} + V(x) \tag{1}$$

acting in the Hilbert space $L_2(\mathbf{R}, H)$, where H is a finite dimensional space, $dimH = m$, potential $V(x)$ is a self-adjoint matrix, bounded and piecewise continuous. We shall investigate relations between the spectral properties of the operators with periodic potential V, $V(x+1) = V(x)$ and cutoff periodic potential $V_N(x) = \begin{cases} V(x), & 0 \leq x \leq N \\ V_0, & x < 0, x > N \end{cases}$, where V_0 is a constant selfadjoint matrix with eigenvalues $\{\lambda_k\}, k = 1, 2, ..., m$ and corresponding eigenvectors $\{e_k\}, k = 1, 2, ..., m$.

The periodic problem has a band structure of the spectrum. The cutoff potential defines an operator with m branches of continuous spectrum $[\lambda_k, \infty)$ and eigenvalues, situated on the half-axis $(-\infty, max\{\lambda_k\}]$. Complete information on the spectrum is accumulated by the scattering and monodromy matrices correspondingly.

The unitary scattering matrix for the second problem can be defined in the following way using the eigenfunctions associated with the energy λ

$$-\frac{\partial^2}{\partial x^2}\Psi(x) + V(x)\Psi(x) = \lambda\Psi(x). \tag{2}$$

These eigenfunctions are combinations of plane waves on the left and right

half axes

$$\Psi(\lambda,x)=\sum_j A_{inc}^{-j}\frac{\exp(\imath\sqrt{\lambda-\lambda_j}x)e_j}{\sqrt[4]{\lambda-\lambda_j}}+\sum_j A_{out}^{-j}\frac{\exp(-\imath\sqrt{\lambda-\lambda_j}x)e_j}{\sqrt[4]{\lambda-\lambda_j}}, x<0;$$

$$\Psi(\lambda,x)=\sum_j A_{inc}^{+j}\frac{\exp(-\imath\sqrt{\lambda-\lambda_j}(x-n))e_j}{\sqrt[4]{\lambda-\lambda_j}}+\sum_j A_{out}^{+j}\frac{\exp(\imath\sqrt{\lambda-\lambda_j}(x-n))e_j}{\sqrt[4]{\lambda-\lambda_j}}, x>n. \tag{3}$$

One can separate two orthogonal sets of eigenfunctions: left incoming waves $A_{inc}^{+}=0$ and right incoming waves $A_{inc}^{-}=0$, parameterized by the amplitudes A_{inc}^{-} and A_{inc}^{+} respectively. The number of the linearly independent eigenfunctions is thus determined by the number of the opened channels , which in turn depends on the energy. The dimension of the S-matrix $\begin{pmatrix} A_{out}^{+} \\ A_{out}^{-} \end{pmatrix} = S \begin{pmatrix} A_{inc}^{+} \\ A_{inc}^{-} \end{pmatrix}$ depends on the energy. The S-matrix disintegrates into the $m\times m$ matrices of reflection and transition coefficients in the case of potential symmetric with respect to the center of the period: $V(1/2+x)=V(1/2-x), x<1/2$:

$$S=\begin{pmatrix} R & T \\ T & R \end{pmatrix}. \tag{4}$$

The unitarity of the scattering matrix can be expressed by the following relations

$$RR^*+TT^*=1,\ RT^*+TR^*=0. \tag{5}$$

The monodromy matrix $\mathcal{M}(\lambda)$ for the periodic problem is defined through the solutions of the equation (2) with periodic potential by the following equality:

$$\begin{pmatrix} \{u^j\}_{j=1}^N \\ \left\{\frac{\partial u^j}{\partial x}\right\}_{j=1}^N \end{pmatrix}|_{x=m+1}=\mathcal{M}(\lambda)\begin{pmatrix} \{u^j\}_{j=1}^N \\ \left\{\frac{\partial u^j}{\partial x}\right\}_{j=1}^N \end{pmatrix}|_{x=m} \tag{6}$$

The band spectrum of the operator is defined by the condition $|Tr\mathcal{M}(\lambda)|<2$.

In order to calculate the scattering matrix from the monodromy matrix we need to introduce the matrix $Q(\lambda)$, which calculates Cauchy data for the set of plane waves from it's amplitudes

$$Q(\lambda)=\begin{pmatrix} (\lambda-\lambda_1)^{-1/4}(e_1), & ..., & (\lambda-\lambda_1)^{-1/4}(e_m), & (\lambda-\lambda_1)^{-1/4}(e_1), & ... \\ (\lambda-\lambda_1)^{1/4}(e_1), & ..., & (\lambda-\lambda_1)^{1/4}(e_m), & -(\lambda-\lambda_1)^{1/4}(e_1), & ... \end{pmatrix}. \tag{7}$$

The monodromy matrix in the representation of plane waves is then given by

$$\tilde{\mathcal{M}}(\lambda) = Q^{-1}(\lambda)\mathcal{M}(\lambda)Q(\lambda). \tag{8}$$

The corresponding power of the matrix connects amplitudes of incoming and outgoing waves:

$$\tilde{\mathcal{M}}^N \begin{pmatrix} A_-^{inc} \\ A_-^{out} \end{pmatrix} = \begin{pmatrix} A_+^{out} \\ A_+^{inc} \end{pmatrix}$$

Above the threshold we thus have :

$$\tilde{\mathcal{M}}^N(\lambda) = Q^{-1}(\lambda)\mathcal{M}^N(\lambda)Q(\lambda) = \begin{pmatrix} T - RT^{-1}R & RT^{-1} \\ -T^{-1}R & T^{-1} \end{pmatrix}. \tag{9}$$

The equalities (9) give us a possibility to calculate the scattering matrix.

Let us examine the relations between the spectra of infinite and finite crystals in the limit of large number N. This question was earlier considered in the papers [6,9], where the ordinary one-dimensional Schrödinger equation was studied. Above the energy barrier $\lambda > \lambda_k$ on each zone of the crystal the special points μ_m were marked. These points divide the zone into N equal sectors in the quasimomentum scale $t(\mu_m) = 2\pi m/N, m = 1, 2, ..., N-1$. The reflection coefficient for the ordinary one-dimensional equation is equal to zero at these points. One can thus see that if the number of periods of the cutoff potentials increases then the number of such points on each band increases also.

For the many mode crystal the corresponding degree of the monodromy matrix has the eigenvalue 1 at these points. Reflection and transition coefficients satisfy the following relations at the marked points μ_m only

$$det(1 - T - R) = 0, \;\; det(1 - T + R) = 0. \tag{10}$$

The equalities (10) define reflectionless scattering matrix in the case of single mode crystal. In the multichannel case only some sets of the plane waves cross the finite crystal without reflection. Multiplicity of the zeroes of the determinants coincides with the multiplicity of the band spectrum.

2.2 Micro spectral properties and band structure

Relations between the spectral properties of the isolated centers forming the crystal and it's band structure is investigated in this subsection using

exactly solvable model. Model problem for the many-mode one-dimensional crystal with the point interaction at some point x_0 is the differential equation $\left(-\frac{\partial^2}{\partial x^2}+V_0\right)\psi(\lambda,x)=\lambda\psi(\lambda,x)$ with the boundary conditions

$$u(x_0-0)=u(x_0+0)=D(\lambda)[\frac{\partial u}{\partial x}](x_0) \tag{11}$$

where $[*](x)$ denotes the jump of the function at point x, $D(\lambda)$ is $m\times m$ matrix with the positive imaginary part in $\Im\lambda>0$, selfadjoint on the real line (so-called R-operator). These boundary conditions depend on the energy λ of the eigenfunction and do not define an operator in the space $L_2(\mathbf{R},H)$. Rigorous operator theory formulation of the problem can be done using self-adjont extensions of the operator with some extra channel of interaction (see [4,5,7,8]). Following ansatz can be used for the discrete spectrum eigenfunction, corresponding to the energy $\lambda=-\chi^2$

$$\psi_j(x)=c_je^{\imath\sqrt{\lambda-\lambda_j}|x-x_0|},\Im\sqrt{\lambda-\lambda_j}>0.$$

Dispersion equation on the energy is obtained from the boundary conditions

$$det\left(diag\{2\imath\sqrt{\lambda-\lambda_j}\}-D^{-1}(\lambda)\right)=0. \tag{12}$$

Negative singularities of the matrix $D(\lambda)$ produce eigenvalues of the problem. Some extra eigenvalues can be formed close to the zero energy.

Unitary scattering matrix can be calculated in the same way. The reflection and transition coefficients for $x_0=0$ are

$$R(k)=\frac{1}{2\imath diag\{\sqrt[4]{\lambda-\lambda_j}\}D(\lambda)diag\{\sqrt[4]{\lambda-\lambda_j}\}-1}, \tag{13}$$

$$T(k)=\frac{2\imath diag\{\sqrt[4]{\lambda-\lambda_j}\}D(\lambda)diag\{\sqrt[4]{\lambda-\lambda_j}\}}{2\imath diag\{\sqrt[4]{\lambda-\lambda_j}\}D(\lambda)diag\{\sqrt[4]{\lambda-\lambda_j}\}-1}. \tag{14}$$

Model of the periodic structure in one-dimensional space can be obtained considering the same differential equation with the boundary conditions (11) at the points $x_n=n-1/2, n=0,\pm1,\pm2,...$ The monodromy matrix can be expressed in terms of the free monodromy matrix $\mathcal{M}_0$ and the jump matrix $J(\lambda)$, corresponding to the single point x_j

$$\mathcal{M}(\lambda)=\mathcal{M}_0^{1/2}(\lambda)J(\lambda)\mathcal{M}_0^{1/2}(\lambda). \tag{15}$$

The matrices $\mathcal{M}_0(\lambda)$ and $J(\lambda)$ are

$$\mathcal{M}_0(\lambda) = \begin{pmatrix} diag(\cos\sqrt{\lambda-\lambda_j}) & diag(\sin\sqrt{\lambda-\lambda_j}/\sqrt{\lambda-\lambda_j}) \\ diag(\sqrt{\lambda-\lambda_j}\sin\sqrt{\lambda-\lambda_j}) & diag(\cos\sqrt{\lambda-\lambda_j}) \end{pmatrix},$$

$$J(\lambda) = \begin{pmatrix} 1 & 0 \\ D^{-1}(\lambda) & 1 \end{pmatrix},$$

where 1 is the unit $m \times m$ matrix. As usual

$$det\mathcal{M}(\lambda) = detJ(\lambda)det\mathcal{M}_0(\lambda) = 1.$$

The spectrum of the problem is purely continuous, it has a band structure. The dispersion equation connects the quasimomentum and the energy of eigenfunctions:

$$det\left(diag\left\{\frac{\sqrt{\lambda-\lambda_j}}{\sin\sqrt{\lambda-\lambda_j}}2(\cos t - \cos\sqrt{\lambda-\lambda_j})\right\} - D^{-1}(\lambda)\right) = 0. \qquad (16)$$

Projecting the surfaces of solutions on the energy axis we obtain the band spectrum.

For one-mode crystal the dispersion equation reads

$$D(k^2)\frac{k}{\sin k}2(\cos t - \cos k) = 1.$$

where $\lambda_1 = 0$, $D(\lambda)$ is an R-function. Solutions of the dispersion equation in the limit of weak connection are situated near the zero-lines of the functions $D(\lambda)$ and $D^{ex}(\lambda, t) \equiv \frac{k}{\sin k}2(\cos t - \cos k), k = \sqrt{\lambda}$. The spectrum of the problem consists of infinitely many bands. Narrow gaps can be observed near the points $\lambda = n^2\pi^2, n = 1, 2, 3, ...$ and zeroes of the function $D(\lambda)$. Only narrow bands occur below the threshold. Every such band corresponds to an eigenvalue of the isolated center. Each positive eigenvalue of the internal operator produces a narrow gap in the band spectrum in the energy scale.

Similar investigation can be carried out in the case of the two mode crystal. Assume that the operator $D(\lambda)$ is of the form

$$D(\lambda) = \begin{pmatrix} D_1 + D_2 & D_1 - D_2 \\ D_1 - D_2 & D_1 + D_2 \end{pmatrix},$$

where $D_{1,2}(\lambda)$ are R-functions. The dispersion equation is:

$$1-(D_1+D_2)(D_1^{ex}+D_2^{ex})+4D_1D_2D_1^{ex}D_2^{ex}=0,$$

$$D_j^{ex}=\frac{\sqrt{\lambda-\lambda_j}}{\sin\sqrt{\lambda-\lambda_j}}2(\cos t-\cos\sqrt{\lambda-\lambda_j}).$$

Zeroes of the external dispersion functions are situated on the parabolas $t=\pm\sqrt{\lambda-a_j}+2\pi m, m\in\mathbf{Z}$. Crossings of these zero lines of the external dispersion functions produce additional gaps in the continuous spectrum.

3 One dimensional chain in the three dimensional space

3.1 Isolated Center

The model problem will be constructed in the same way as in the previous subsection. Laplace operator in $L_2(\mathbf{R}^3)$ can be defined on the set of smooth functions with the following singularity at one point x_0:

$$\Psi(x)\sim\frac{\Psi_-}{4\pi|x-x_0|}+\Psi_0+o(1), x\to x_0, \Psi_-,\Psi_0\in\mathbf{C}. \tag{17}$$

We consider the energy dependent boundary conditions

$$\Psi_-/\Psi_0=D(\lambda), \tag{18}$$

with R-function $D(\lambda)$. The first model of this type with the real constant D was considered in [1-3]. The following ansatz is valid for the continuous spectrum eigenfunctions

$$\Psi(\vec{k},x)=\frac{1}{\sqrt{2\pi}}\left(e^{\imath<\vec{k},\vec{x}>}+\frac{D(k^2)}{1-\frac{\imath k}{4\pi}D(k^2)}\frac{e^{\imath k|x-x_0|}}{4\pi|x-x_0|}\right), k=\sqrt{\lambda} \tag{19}$$

The scattering matrix and the eigenstate dispersion equation are

$$S(\lambda)=\frac{\frac{\imath k}{4\pi}+D^{-1}(k^2)}{\frac{\imath k}{4\pi}-D^{-1}(k^2)},\quad \frac{\imath k}{4\pi}=D^{-1}(k^2) \tag{20}$$

Every negative zero of $D(\lambda)$ produces eigenvalue of the operator, while the positive zeroes define resonances - singularities of S-matrix on non-physical sheet of the energy.

3.2 One-dimensional Chain.

The following model for a one-dimensional chain in three-dimensional space will be considered. We impose boundary conditions of the type (18) at the points : $x_j = j\vec{e}, j \in \mathbf{Z}$, where $\vec{e}$ is vector of the period of the chain. The spectrum is purely continuous, corresponding to scattered waves and waveguide functions. Eigenfunctions of the first type describe process of the scattering on the chain and contain an incoming plane wave. Waveguide functions describe transport along the chain and define the band spectrum of the operator. These eigenfunctions can be written in the Bloch representation with the quasimomentum t :

$$\Phi(t,x) = \sum_{j\in\mathbf{Z}} \frac{e^{\imath k|x-x_j|}}{4\pi|x-x_j|} e^{\imath jt}. \tag{21}$$

The energy and the quasimomentum are connected by the dispersion equation

$$D^{-1}(E) = \tilde{B}(k,t) \equiv \frac{\imath k}{4\pi} + \sum_{j\neq 0} \frac{e^{\imath k|x_j|}}{4\pi|x_j|} e^{\imath tj} \equiv \frac{1}{4\pi} \ln \frac{1}{2(\cos k - \cos t)} \tag{22}$$

Solutions of the equation (22) are situated in the region $E < 0$ or $t > |k|$. Narrow gaps in the spectrum are obtained near the zeroes of D, which corresponds to the resonances of the isolated center. Eigenstates of the isolated center produce small bands of continuous spectrum of the chain.

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