ELECTRON IN A HOMOGENEOUS CRYSTAL OF POINT ATOMS WITH INTERNAL STRUCTURE. II

P. B. Kurasov and B. S. Pavlov

A spectral analysis is made of a Schrödinger operator with zero-range potential of the type of a one- or two-dimensional lattice in the presence of internal structure. The relationship between the resonances of an isolated atom and the spectral properties of the crystal is established.

In the first part of the present work [1], the following problem was solved in a model situation: How does the presence of resonances of the isolated atom affect the spectrum of the corresponding crystal? It was found that sharp resonances at least can lead to the appearance of gaps in the bands of the continuum of the corresponding crystal and will in all cases lead to changes in the multiplicity of the spectrum, specifically, to the disappearance of some Bloch waves. The method of zero-range potentials with internal structure used in [1] can also be applied to the corresponding problem of one- and two-dimensional crystals in R^3. This problem was solved earlier in [2], as was pointed out to the authors by V. M. Borodin. The translation of the results of [2] into a rigorous language requires analysis in a Hilbert space with indefinite metric. In contrast to this, the approach that employs zero-range potentials with internal structure brings out the connection between the resonances of an isolated atom and the structure in the spectrum of a one-dimensional chain (or two-dimensional lattice) at the level of explicit formulas already in an ordinary Hilbert space of the form $L_2(R^3)\oplus E$ with finite-dimensional orthogonal auxiliary E. We show that the presence of resonances in the isolated atom leads to the appearance in the spectrum of the crystal of gaps in real waveguide bands and, in agreement with [2], to the appearance of resonance bands; we also describe their localization under the condition that the resonances are made sharp. These bands are situated on the unphysical sheet, sometimes directly below the real ("physical") bands of waveguide type, to which there correspond Bloch functions quasiperiodic along the chain (lattice) and decreasing with increasing distance from it. Besides these bands, the spectrum of the one-dimensional (two-dimensional) crystal in R^3 contains a real branch $(0, \infty)$, to which there correspond scattered waves parametrized by unit vectors in R^3; this branch is completely analogous to the corresponding branch in the spectrum of the Laplacian.

1. Laying down in R^3 a one- or two-dimensional lattice

$$\mathbf{x}_n=n\mathbf{e},\ n=0,\pm1,\pm2,\dots\ (\mathbf{x}_n=n^1\mathbf{e}_1+n^2\mathbf{e}_2,\ n^i=0,\pm1,\pm2,\dots),$$

along the vector $\mathbf{e}$ (respectively, in the plane $(\mathbf{e}_1,\mathbf{e}_2)$), we form the orthogonal sum $L_2(R^3)\oplus\sum E_n$ of the space of all square-summable functions in R^3 and a countable number of auxiliary spaces E_n, which, in the simplest case, we shall assume are identical: $E_n = E_0$. We shall assume that on each of the spaces E_n there acts the operator A_n. Having in mind the construction of a model of a homogeneous crystal, we shall assume here that $A_n = A_0$. Without loss of generality, it can be assumed that the operator A_0 has a simple spectrum. We restrict each of the operators A_n to a symmetric operator A_n^0 with deficiency index (1, 1) in such a way that the deficiency element φ is a generating element, and we form a boundary form* corresponding to it for $\xi_n,\eta_n\in D(A_n^{0*})$:

$$\langle A_n^{0*}\xi_n,\eta_n\rangle-\langle\xi_n,A_n^{0*}\eta_n\rangle=\xi_{n1}\overline{\eta_{n0}}-\xi_{n0}\overline{\eta_{n1}}=[\xi_n,\eta_n]_n.$$

*In the case when the domain of definition of the restricted operator is not dense in E_n, one can also form a boundary form with analogous properties [3].

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It is symplectic in the space of boundary values $\{\xi_{n0}, \xi_{n1}\}$ of elements ξ in $D(A^{0*})$. To the operator $A_{in}{}^0 = \oplus\sum A_n{}^0$ there corresponds the total boundary form

$$\sum [\xi_n, \eta_n]_n = [\xi_\partial, \eta_\partial]^{in},$$

whose arguments are infinite vectors of boundary values $\xi_\partial = \left\{\begin{pmatrix}\xi_{n0}\\ \xi_{n1}\end{pmatrix}\right\}_{n=-\infty}^{\infty}$. We denote the infinite-dimensional space of these vectors by E_∂^{in}.

Besides the symmetric operator A_{in}^0, we also consider the symmetric restriction $-\Delta^0$ of the Laplacian in R^3 to the set of all smooth functions that vanish near the points x_n of the lattice. Elements in the domain of definition of the adjoint operator have near the points x_n an asymptotic behavior whose coefficients have the meaning of boundary values:

$$u(x) = \frac{u_{n-}}{4\pi|x-x_n|} + u_{n0} + o(1).$$

The boundary form corresponding to this restriction is also symplectic in the space E_∂^{ext} of infinite-dimensional boundary vectors $U_\partial = \left\{\begin{pmatrix}u_{n0}\\ u_{n-}\end{pmatrix}\right\}_{n=-\infty}^{\infty}$:

$$\langle(-\Delta^0)^* u, v\rangle - \langle u, (-\Delta^0)^* v\rangle = \sum_n (u_{n0}\bar{v}_{n-} - u_{n-}\bar{v}_{n0}) = [U_\partial, V_\partial]^{ext}.$$

Our immediate aim is to describe the self-adjoint extensions of the symmetric operator $A_{in}{}^0 \oplus (-\Delta^0)$, which has infinite deficiency indices. As in the case of finite deficiency indices (see [3]), the matter reduces to separating in the boundary space of maximal neutral subspaces N the total boundary form:

$$[\xi, \eta]^{in} + [U_\partial, V_\partial]^{ext} = 0; \quad (U_\partial, \xi), (V_\partial, \eta) \in N.$$

Membership of the boundary vectors of the element (U, ξ) to a given maximal neutral subspace N (Lagrangian plane) fixes the self-adjoint boundary condition that determines the self-adjoint extension $\mathscr{L}_N$ of the symmetric operator $A_{in}{}^0 \oplus (-\Delta^0)$. For convenience of the reader, we give here without proof the general description of self-adjoint boundary conditions.

Let $J[\xi, \eta]$ be the symplectic form on the Hilbert space H defined on the orthogonal decomposition $H = E_0 \oplus E_1$ by the Bloch matrix $J = \begin{pmatrix} 0 & I\\ -I & 0\end{pmatrix}$. The subspaces E_0 and E_1 can be assumed to be identical: $E_0 = E_1 = E$. Then vectors ξ in H can be expressed in two-component form (ξ_0, ξ_1), and $J[\xi, \eta] = \langle\xi_1, \eta_0\rangle - \langle\xi_0, \eta_1\rangle$. The eigenspaces of the matrix J corresponding to the eigenvalues $\pm i$ consist of vectors of the form $\left\{\begin{pmatrix}1\\ i\end{pmatrix}h\right\}, \left\{\begin{pmatrix}i\\ 1\end{pmatrix}g\right\}$, respectively, and every isometry $\tilde{V}$ from N_+ to N_- is uniquely determined by a unitary operator V that acts on E:

$$\tilde{V}\left\{\begin{pmatrix}i\\ 1\end{pmatrix}g\right\} = \left\{\begin{pmatrix}1\\ i\end{pmatrix}Vg\right\}. \tag{1}$$

<u>PROPOSITION 1.</u> The family of all maximal neutral subspaces of the symplectic form can be described by any of the three following equivalent ways.

1. Let $\tilde{V}$ be an arbitrary isometry from N_+ to N_-. Then to it there corresponds the neutral subspace $L_V = (I + \tilde{V})N_+$, and every neutral subspace can be obtained in this way (up to a J-unitary transformation).

2. Let F_s, $s = 0, 1$, be any orthogonal subspaces in E (one or both of them may be trivial), $G = E\ominus[F_0 \oplus F_1]$ be their orthogonal complement, and A be a self-adjoint operator on G. Then the closure of every lineal in H distinguished by the boundary conditions $\xi_0 = f_1 + g$, $f_1 \in F_1$, $g \in D(A)$; $\xi_1 = f_0 + Ag$, $f_0 \in F_0$, or $\xi_0 = f_1 + Ag$, $f_1 \in F_1$; $\xi_1 = f_0 + g$, $f_0 \in F_0$, $g \in D(A)$, is a neutral subspace, and every neutral subspace can be obtained in this way up to a J-unitary transformation.

3. Let A be an arbitrary self-adjoint operator on E. Then the closures in H of the lineals distinguished by the boundary conditions $\xi_0 = A\xi_1$ or $\xi_1 = A\xi_0$ are neutral subspaces

in H. All the neutral subspaces can be obtained in this way up to a J-unitary transformation.

Description 3 corresponds to the usual description of Lagrangian planes in terms of generating functions except for the replacement of the bilinear forms by the corresponding operators. We note that the simplest J-unitary transformation is $(\xi_0, \xi_1)\to(-\xi_1, \xi_0)$. Therefore, to construct self-adjoint extensions of the operator $A_{1n}{}^0\oplus(-\Delta^0)$, we shall in what follows use two types of boundary condition ensuring homogeneity of the crystal:

$$(\Gamma):\begin{pmatrix}\vdots\\ \begin{pmatrix}u_{n0}\\ \xi_{n1}\end{pmatrix}\\ \vdots\end{pmatrix}=(n)\begin{pmatrix} & (n) & \\ & \vdots & \\ \ldots & \Gamma_2{}^*\Gamma_1{}^*\Gamma_0\Gamma_1\Gamma_2 & \ldots\\ & \vdots & \\ & (n) & \end{pmatrix}\begin{pmatrix}\vdots\\ \begin{pmatrix}u_{n-}\\ \xi_{n0}\end{pmatrix}\\ \vdots\end{pmatrix},$$

$$(\mathrm{B}):\begin{pmatrix}\vdots\\ \begin{pmatrix}u_{n0}\\ \xi_{n0}\end{pmatrix}\\ \vdots\end{pmatrix}=(n)\begin{pmatrix} & (n) & \\ & \vdots & \\ \ldots & \mathrm{B}_2{}^*\mathrm{B}_1{}^*\mathrm{B}_0\mathrm{B}_1\mathrm{B}_2 & \ldots\\ & \vdots & \\ & (n) & \end{pmatrix}\begin{pmatrix}\vdots\\ \begin{pmatrix}u_{n-}\\ -\xi_{n1}\end{pmatrix}\\ \vdots\end{pmatrix}.$$

We shall assume that the infinite Hermitian matrices Γ and B that determine the extensions are Toeplitz matrices, $B_s = B_s^*$; moreover, we shall limit ourselves to taking into account the interaction of only the nearest neighbors: $B_s = \Gamma_s = 0$, $|s| > M$. By virtue of Part 3 of Proposition 1 the conditions (Γ) and (B) (together with the analogous conditions in which the matrices Γ and B occur on the left) exhaust all self-adjoint extensions $A_{1n}{}^0\oplus(-\Delta^0)$ corresponding to homogeneous crystals in which overlapping of the atomic orbitals of only the nearest neighbors is taken into account. Further, we consider only extensions corresponding to the matrices

$$\mathrm{B}_l=\begin{pmatrix}0&0\\0&\beta_l\end{pmatrix}=\mathrm{B}_{-l}{}^*,\quad \Gamma_l=\begin{pmatrix}0&0\\0&\gamma_l\end{pmatrix}=\Gamma_{-l}{}^*,\quad 0<|l|<M,$$

$$\mathrm{B}_0=\begin{pmatrix}\beta_{00}&\beta_{01}\\ \bar\beta_{01}&\beta_{11}\end{pmatrix},\quad \Gamma_0=\begin{pmatrix}\gamma_{00}&\gamma_{01}\\ \bar\gamma_{01}&\gamma_{11}\end{pmatrix},\quad \operatorname{Im}\beta_{ii}=\operatorname{Im}\gamma_{ii}=0.$$

2. The operators $\mathscr{L}_\Gamma$, $\mathscr{L}_B$ that are the self-adjoint extensions of $A_{1n}{}^0\oplus(-\Delta^0)$ with the boundary conditions Γ and B have a purely continuous spectrum consisting of two branches. First, there are scattered waves parametrized by a unit vector $\mathbf{v}\neq\mathbf{e}_s$. Their components in the external and internal spaces have the form

$$\Psi_\mathbf{v}(\mathbf{x},k)=e^{-ik\langle\mathbf{x},\mathbf{v}\rangle}+\sum_{(\mathbf{n})}\frac{e^{ik|\mathbf{x}-\mathbf{n}|}}{4\pi|\mathbf{x}-\mathbf{n}|}e^{-ik\langle\mathbf{n},\mathbf{v}\rangle}\rho(\boldsymbol{\tau}),\quad \xi_n{}^\Psi=\xi_0{}^\Psi e^{-ik\langle\mathbf{n},\mathbf{v}\rangle},\quad \mathbf{n}=n^1\mathbf{e}_1+n^2\mathbf{e}_2,\quad n^s=0,\ \pm1,\ \pm2,\ldots. \tag{2}$$

Second, there are Bloch waves

$$\varphi(\mathbf{x},k)=\sum_{(\mathbf{n})}\frac{e^{ik|\mathbf{x}-\mathbf{n}|}}{4\pi|\mathbf{x}-\mathbf{n}|}e^{-i\langle\mathbf{n},\mathbf{t}\rangle},\quad \xi_n{}^\varphi=\xi_0{}^\varphi e^{-i\langle\mathbf{n},\mathbf{t}\rangle},\quad \mathbf{n}=n^1\mathbf{e}_1+n^2\mathbf{e}_2,\quad n^s=0,\ \pm1,\ \pm2,\ldots. \tag{3}$$

The connection between the spectral parameter $\lambda = k^2$ and the quasimomenta $\boldsymbol{\tau}$ and $\mathbf{t}$ of the scattered waves Ψ_ν and the eigenfunctions of waveguide type are determined from the boundary conditions

$$(\Gamma,\Psi):\begin{pmatrix}\rho\frac{ik}{4\pi}+1+\rho\sum\limits_{\mathbf{n}\neq0}\frac{e^{ik|\mathbf{n}|}}{4\pi|\mathbf{n}|}e^{-ik\langle\mathbf{n},\mathbf{v}\rangle}\\ \xi_1\end{pmatrix}=\begin{pmatrix}\gamma_{00}&\gamma_{01}\\ \bar\gamma_{01}&\gamma_{11}\end{pmatrix}\begin{pmatrix}\rho\\ \xi_0\end{pmatrix}+\begin{pmatrix}0\\ \sum\limits_{1<|\mathbf{l}|<M}\gamma_l e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\xi_0\end{pmatrix};$$

$$(B,\Psi):\begin{pmatrix}\rho\frac{ik}{4\pi}+1+\rho\sum\limits_{n\neq0}\frac{e^{ik|\mathbf{n}|}}{4\pi|\mathbf{n}|}e^{-ik\langle\mathbf{n},\mathbf{v}\rangle}\\ \xi_0\end{pmatrix}=\begin{pmatrix}\beta_{00}&\beta_{01}\\ \bar\beta_{01}&\beta_{11}\end{pmatrix}\begin{pmatrix}\rho\\ -\xi_1\end{pmatrix}+\begin{pmatrix}0\\ -\sum\limits_{1<|\mathbf{l}|<M}\beta_l e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\xi_1\end{pmatrix};$$

$$(\Gamma,\ \varphi):\ \begin{pmatrix} \frac{ik}{4\pi}+\sum_{\mathbf{n}\neq 0}\frac{e^{ik|\mathbf{n}|}}{4\pi|\mathbf{n}|}e^{-i\langle\mathbf{n},\,\mathbf{t}\rangle} \\ \xi_1 \end{pmatrix}=\begin{pmatrix}\gamma_{00} & \gamma_{01}\\ \overline{\gamma_{01}} & \gamma_{11}\end{pmatrix}\begin{pmatrix}1\\ \xi_0\end{pmatrix}+\begin{pmatrix}0\\ \sum_{1<|\mathbf{l}|<M}\gamma_{\mathbf{l}}e^{-i\langle\mathbf{l},\,\mathbf{t}\rangle}\xi_0\end{pmatrix};$$

$$(B,\ \varphi):\ \begin{pmatrix} \frac{ik}{4\pi}+\sum_{\mathbf{n}\neq 0}\frac{e^{ik|\mathbf{n}|}}{4\pi|\mathbf{n}|}e^{-i\langle\mathbf{n},\,\mathbf{t}\rangle} \\ \xi_0 \end{pmatrix}=\begin{pmatrix}\beta_{00} & \beta_{01}\\ \overline{\beta_{01}} & \beta_{11}\end{pmatrix}\begin{pmatrix}1\\ -\xi_1\end{pmatrix}+\begin{pmatrix}0\\ -\sum_{1<|\mathbf{l}|<M}\beta_{\mathbf{l}}e^{-i\langle\mathbf{l},\,\mathbf{t}\rangle}\xi_1\end{pmatrix}.$$

Here, we denote by $\mathbf{l}$ the integral vector $l^1\mathbf{e}_1+l^2\mathbf{e}_2$ in the case of the two-dimensional lattice, or the vector $l\mathbf{e}$ in the case of a one-dimensional lattice.

Solving these equations, we must use the fact that the boundary values of the elements ξ_n of the internal subspaces that belong to the domain of definition of A^{0*} are connected by the relation (see [3])

$$\xi_1\xi_0^{-1}=\langle(A-\lambda I)^{-1}(I+\lambda A)\varphi,\ \varphi\rangle_H\equiv\Delta(\lambda).$$

On the right-hand side here we have the Schwartz integral of the operator A on the deficiency element φ. This enables us to find the external and internal components of the scattered waves in terms of lattice sums,

$$\gamma_{2,1}(k,\boldsymbol{\tau})=\frac{ik}{4\pi}+\sum_{\mathbf{n}\neq 0,\ \mathbf{n}\in\mathbb{Z}^2,\ \mathbb{Z}^1}\frac{e^{ik|\mathbf{n}|}}{4\pi|\mathbf{n}|}e^{-i\langle\mathbf{n},\,\boldsymbol{\tau}\rangle},\quad \boldsymbol{\tau}=k\mathbf{v}, \tag{4}$$

and the external and internal components of the eigenfunctions of waveguide type in terms of the same lattice sums with the parameter $\boldsymbol{\tau}$ replaced by the quasimomentum $\mathbf{t}$. In the case of the one-dimensional lattice, the lattice sums are calculated in explicit form:

$$\gamma_1(k,\mathbf{t})=\frac{ik}{4\pi}+\sum_{n\neq 0,\ n\in\mathbb{Z}}^{1}\frac{e^{ik|n|}}{4\pi|n|}e^{-int}=\frac{1}{4\pi}\ln\frac{1}{2(\cos k-\cos t)}.$$

Here, the branch of the logarithm is fixed by the condition which ensures that $\gamma_1(k,\ t)$ can be continued analytically into the upper half-plane Im $k > 0$. The imaginary part of the function γ_1 is piecewise constant and in the strip $|t|<\pi$, $-\infty<k<\infty$ takes values that are multiples of 1/4 (see Fig. 1). The real part has logarithmic singularities on the lines $k \pm t = 2\pi n$, $n = 0 \pm 1, \ldots$, i.e., becomes $+\infty$ on them. On the ovals $\cos k - \cos t = \pm 1/2$ we have Re $\gamma_1 = 0$, and within the ovals Re $\gamma_1 < 0$. For complex k with small imaginary part, $\gamma_1(k,\ t)$ can be calculated in accordance with the formula

$$\gamma_1(k,\mathbf{t})\approx\gamma_1(\operatorname{Re}k,\mathbf{t})+\frac{1}{4\pi}\frac{\sin(\operatorname{Re}k)}{\cos(\operatorname{Re}k)-\cos t}i\operatorname{Im}k. \tag{5}$$

For purely imaginary k, corresponding to negative values of the energy, $\lambda < 0$, the function γ_1 is real and smooth. It decreases monotonically, tending to $-\infty$.

The lattice sum $\gamma_2(k,\mathbf{t})$ cannot be calculated explicitly. Nevertheless, its properties have been fairly well studied in [4], in which, in particular, it was shown that:

1. For fixed value of the spectral variable k $\gamma_2(k,\ \mathbf{t})$ is an even function of each of the components $(t^1,\ t^2)$ of the quasimomentum.

2. With respect to the spectral variable $\lambda = k^2$ the function is analytic and has positive imaginary part in the upper half-plane and a cut on the half-axis $|\mathbf{t}|^2<\lambda<\infty$, on the upper edge of which $\operatorname{Im}\gamma_2(\lambda,\mathbf{t})>0$. On the half-axis $-\infty<\lambda<|\mathbf{t}|^2$ the function $\gamma_2(\lambda,\mathbf{t})$ is real and increases monotonically from $-\infty$ to $+\infty$.

3. On the half-axis $-\infty<\lambda<|\mathbf{t}|^2$

$$\frac{\partial\gamma_2}{\partial t^i}=-\sin t^i\cdot f_i(\lambda,\mathbf{t}),$$

where $f_i(\lambda,\mathbf{t})$ are smooth strictly positive functions.

4. $\gamma_2(0,\ \pi,\ \pi) < 0$.

5. The derivative $\partial\gamma_2/\partial\gamma$ has the representation

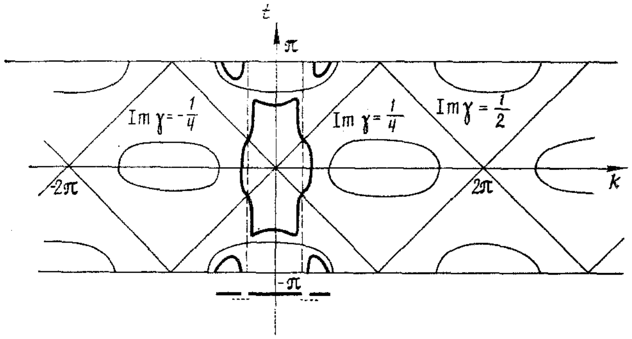

Fig. 1

$$\frac{\partial\gamma_2}{\partial\lambda}=\frac{1}{4}\sum_{\mathbf{n}\in\mathbb{Z}^2}(|2\pi\mathbf{n}+\mathbf{t}|^2-\lambda)^{-3/2},\quad \lambda=k^2,$$

where the branches of the roots are chosen to satisfy the condition $\operatorname{Im}\gamma_2\cdot\operatorname{Im}\lambda \geqq 0$.

It follows from properties 1-5 in particular that in the cylinder $|t^1, t^2|<\pi$, $-\infty<k<\infty$ the function γ_2 is real for $0<k<|\mathbf{t}|$, and, further, on the passage through the surface on which $k^2=|2\pi\mathbf{n}+\mathbf{t}|^2$, it does not, in contrast to γ_1, have a discontinuity but acquires additional singularities corresponding to the corresponding terms in Eq. (5):

$$\gamma_2(k^2-|2\pi\mathbf{n}+\mathbf{t}|^2+\delta)-\gamma_2(k^2-|2\pi\mathbf{n}+\mathbf{t}|^2-\delta)\approx\frac{2(i-1)}{\sqrt{\delta}}.$$

The function γ_2 does not have other singularities in the cylinder.

We use the obtained results to construct the scattered waves and eigenfunctions of waveguide type, and also for qualitative investigation of the spectrum.

PROPOSITION 2. The scattered waves corresponding to the boundary conditions Γ and B are determined by formula (2), in which it is necessary to take for the conditions Γ and B, respectively,

$$\rho_\Gamma(k\mathbf{v},\boldsymbol{\tau})=\frac{\Delta+\gamma_{11}-\sum\limits_{1<|\mathbf{l}|<M}\gamma_{l}e^{-ik\langle\mathbf{v},\mathbf{l}\rangle}}{|\gamma_{01}|^2-(\gamma_{00}-\gamma(k,\boldsymbol{\tau}))\Big(\gamma_{11}+\sum\limits_{1<|\mathbf{l}|<M}\gamma_{l}e^{-ik\langle\mathbf{v},\mathbf{l}\rangle}-\Delta\Big)}$$

$$\rho_B(k\mathbf{v},\boldsymbol{\tau})=-\frac{1+\Delta\Big(\beta_{11}+\sum\limits_{1<|\mathbf{l}|<M}\beta_{l}e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\Big)}{|\beta_{01}|^2\Delta-(\beta_{00}-\gamma(k,\mathbf{t}))\Big(1+\Delta\Big(\beta_{11}+\sum\limits_{1<|\mathbf{l}|<M}\beta_{l}e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\Big)\Big)}$$

Here, k = k + i0, and $\boldsymbol{\tau}$ is the projection of the vector $k\mathbf{v}$, which determines the energy and direction of incidence of the plane wave, onto the plane (line) of the lattice. For the eigenfunctions of waveguide type, the dispersion relations connecting the energy k^2 and quasimomentum $\mathbf{t}$ of the electron in the lattice have the form

$$(\Gamma):\qquad (\gamma(k,\mathbf{t})-\gamma_{00})\Big(\Delta-\gamma_{11}-\sum_{1<|\mathbf{l}|<M}\gamma_{l}e^{-i\langle\mathbf{l},\mathbf{t}\rangle}\Big)=|\gamma_{01}|^2;$$

$$(B):\qquad (\gamma(k,\mathbf{t})-\beta_{00})\Big(-\Delta^{-1}-\gamma_{11}-\sum_{1<|\mathbf{l}|<M}\gamma_{l}e^{-i\langle\mathbf{l},\mathbf{t}\rangle}\Big)=|\beta_{00}|^2.$$

Here, as γ in the case of the one- and two-dimensional lattice one must take the corresponding lattice sums (4) for ρ or the corresponding sums with quasimomentum for the dispersion relations.

Bearing in mind that for all elements ξ in the domain of definition of A^{0*} the boundary values are related by the equation $\xi_1 = \Delta\xi_0$, we write the equations (Γ) and (Ψ) in the form

$$1+\rho_\Gamma\gamma=\gamma_{00}\rho_\Gamma+\gamma_{01}\xi_0,$$

$$\Delta\xi_0=\bar\gamma_{01}\rho_\Gamma+\gamma_{11}\xi_0+\xi_0\sum_{1<|\mathbf{l}|<M}\gamma_l e^{-ik\langle\mathbf{v},\mathbf{l}\rangle};$$

from which we obtain the value of the parameter ρ_Γ in the formula for the scattered wave:

$$1+\rho_\Gamma(\gamma-\gamma_{00})=\frac{|\gamma_{01}|^2\rho_\Gamma}{\Delta-\gamma_{11}-\sum\limits_{1<|\mathbf{l}|<M}\gamma_l e^{-ik\langle\mathbf{v},\mathbf{l}\rangle}},\quad \rho_\Gamma=\frac{\Delta-\gamma_{11}-\sum\limits_{1<|\mathbf{l}|<M}e^{-ik\langle\mathbf{v},\mathbf{l}\rangle}}{|\gamma_{01}|^2-(-\gamma+\gamma_{00})\left(-\Delta+\gamma_{11}+\sum\limits_{1<|\mathbf{l}|<M}\gamma_l e^{-ik\langle\mathbf{v},\mathbf{l}\rangle}\right)}.$$

Everywhere on the right-hand side the values of the analytic functions γ are to be understood as the limiting values as $k \to k + i0$ (from the upper half-plane).

The obtained formula is equally valid for the two- and one-dimensional lattices. It is merely necessary to substitute in it the corresponding lattice sum $\gamma=\gamma(k, \mathbf{k}'')$, where $\mathbf{k}''$ is the projection of the vector $\mathbf{k}$, which determines the direction of incidence of the plane wave, onto the plane (line) of the lattice.

Similarly, for the scattered waves for the boundary condition B we obtain the equations

$$1+\rho_B\gamma=\beta_{00}\rho_B-\beta_{01}\Delta\xi_0,\quad \xi_0=\bar\beta_{01}\rho_B-\beta_{11}\Delta\xi_0-\Delta\xi_0\sum_{1<|\mathbf{l}|<M}\beta_l e^{-ik\langle\mathbf{l},\mathbf{v}\rangle},$$

from which we find the value of ρ_B:

$$1+\rho_B(\gamma-\beta_{00})+|\beta_{01}|^2\Delta\rho_B\left[1+\Delta\left(\beta_{11}+\sum_{1<|\mathbf{l}|<M}\beta_l e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\right)\right]^{-1}=0,$$

$$\rho_B=-\frac{1+\Delta\left(\beta_{11}+\sum\limits_{1<|\mathbf{l}|<M}\beta_l e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\right)}{(\gamma-\beta_{00})\left[1+\Delta\left(\beta_{11}+\sum\limits_{1<|\mathbf{l}|<M}e^{-ik\langle\mathbf{l},\mathbf{v}\rangle}\right)\right]+|\beta_{01}|^2\Delta},\qquad k=k+i0.$$

For the eigenfunctions of waveguide type, we obtain the equations

$$(\Gamma,\varphi):\quad \begin{cases}\gamma(k,\mathbf{t})=\gamma_{00}+\gamma_{01}\xi_0,\\ \Delta\xi_0=\bar\gamma_{01}+\gamma_{11}\xi_0+\xi_0\sum\limits_{1<|\mathbf{l}|<M}\gamma_l e^{-i\langle\mathbf{l},\mathbf{t}\rangle},\end{cases}$$

$$(B,\varphi):\quad \begin{cases}\gamma(k,\mathbf{t})=\beta_{00}-\Delta\beta_{01}\xi_0,\\ \xi_0=\bar\beta_{01}-\Delta\xi_0\gamma_{11}-\Delta\xi_0\sum\limits_{1<|\mathbf{l}|<M}\beta_l e^{-i\langle\mathbf{l},\mathbf{t}\rangle}\end{cases}$$

from which we obtain dispersion relations connecting the energy k^2 to the quasimomentum of the electron in the lattice:

$$(\Gamma,\varphi):\quad (\gamma(k,\mathbf{t})-\gamma_{00})\left(\Delta-\gamma_{11}-\sum_{1<|\mathbf{l}|<M}\gamma_l e^{-i\langle\mathbf{l},\mathbf{t}\rangle}\right)=|\gamma_{01}|^2,$$

$$(B,\varphi):\quad (\gamma(k,\mathbf{t})-\beta_{00})\left(1+\Delta\left(\beta_{11}+\sum_{1<|\mathbf{l}|<M}\beta_l e^{-i\langle\mathbf{l},\mathbf{t}\rangle}\right)\right)=-|\beta_{01}|^2\Delta.$$

3. We now study the band structure of the one-dimensional lattice that is generated by the eigenfunctions of waveguide type, making the assumption, for example, that the coupling constants γ_{01} and β_{01} of the external and internal channels are small and that the overlap integrals of the atomic orbitals γ_ℓ and β_ℓ are zero. Having marked in Fig. 1 with the vertical broken lines the roots of the equation $\Delta - \gamma_{11} = 0$ that lie in the interval $[-\pi, \pi]$, we note that in the regions in which $t^2 > k^2$, $|t| < \pi$ we have $\operatorname{Im}\gamma = 0$, and the solutions of the dispersion relation are real and lie near the lines where $\Delta = \gamma_{11}$,

$\gamma = \gamma_{00}$ (however, not on them). But in the regions in which Im $\gamma = \pm 1/4$ the roots of the dispersion relation are complex, and to find them near the discontinuity lines we must use the representation (5),

$$\gamma(k, \mathbf{t}) \approx \operatorname{Re}\gamma(\operatorname{Re} k, \mathbf{t}) \pm \frac{i}{4} + \frac{i}{4\pi}\frac{\sin(\operatorname{Re} k)}{\cos(\operatorname{Re} k) - \cos t}\operatorname{Im} k,$$

which for the boundary conditions Γ gives

$$\left[\operatorname{Re}\gamma(\operatorname{Re} k, \mathbf{t}) - \gamma_{00} + i\left\{\frac{\sin(\operatorname{Re} k)\operatorname{Im} k}{\cos(\operatorname{Re} k) - \cos t} \pm \frac{1}{4}\right\}\right](\Delta - \gamma_{11}) = |\gamma_{01}|^2.$$

$$[\operatorname{Re}\gamma(\operatorname{Re} k, \mathbf{t}) - \gamma_{00}](\Delta - \gamma_{11}) \approx |\gamma_{01}|^2, \quad \operatorname{Im} k = \mp\frac{1}{4}\frac{\cos(\operatorname{Re} k) - \cos t}{\sin(\operatorname{Re} k)}, \quad k^2 \approx t^2.$$

For $\gamma_{00} > 0$, the solutions of the obtained equation are projected onto the k axis in the form of two real bands separated by a gap near the resonance of the isolated atom and next to it a quasistationary band, which is situated below this gap on the unphysical sheet Im $k < 0$:

$$\operatorname{Im} k \approx \mp\frac{1}{4}\frac{\cos(\operatorname{Re} k) - \cos t}{\sin(\operatorname{Re} k)} \qquad (k > 0, k < 0, k^2 > t^2).$$

In all the other regions in which Im $\gamma \neq 0$ there arise only quasistationary bands, corresponding to complex values of the energy. For example, if the line of the root $\Delta - \gamma_{11} = 0$ passes through the point k_0, $\pi < k_0 < 2\pi$, the corresponding dispersion relations have only complex roots. The lines of roots near the straight lines $k \pm t = 2\pi$ are

$$\left[\operatorname{Re}\gamma(\operatorname{Re} k, t) - \gamma_{00} + i\left\{\frac{\sin(\operatorname{Re} k)\operatorname{Im} k}{\cos(\operatorname{Re} k) - \cos t} + \binom{1/4}{1/2}\right\}\right](\Delta - \gamma_{11}) \approx |\gamma_{01}|^2.$$

Here, it is necessary to take the 1/4 or 1/2 in the round brackets in accordance with the value of Im γ in the corresponding region. We obtain

$$\operatorname{Im} k = -\binom{1/4}{1/2}\frac{\cos(\operatorname{Re} k) - \cos t}{\sin(\operatorname{Re} k)}, \qquad k \pm t \approx 2\pi, \quad [\operatorname{Re}\gamma(\operatorname{Re} k, t) - \gamma_{00}](\Delta - \gamma_{11}) \approx |\gamma_{01}|^2.$$

For negative values of λ (imaginary k, Im $k > 0$) the lattice sum γ decreases monotonically as $-\sqrt{|\lambda|}$ at infinity. Therefore, near each negative root of the equation $\Delta(\lambda) - \gamma_{11} = 0$ for small coupling constants $|\gamma_{10}| \ll 1$ there is a narrow band, which is obtained by projecting onto the λ axis the line of roots of the corresponding dispersion relation:

$$[\gamma(\sqrt{\lambda}, t) - \gamma_{00}](\Delta(\lambda) - \gamma_{11}) = |\gamma_{01}|^2.$$

In addition, one further band (in general, a broader one) is generated by the line of roots of the lattice sum $\gamma(\sqrt{\lambda}, t) - \gamma_{00} = 0$. If this band contains a negative eigenstate of the isolated atom, $\Delta(\lambda) - \gamma_{11} = 0$, then near it there arises a narrow gap in the same way as occurs in a three-dimensional crystal.

In the case of the two-dimensional lattice, the picture of the real bands generated by the "lattice" band $\{\lambda : \gamma_2(\sqrt{\lambda}, \mathbf{t}) - \gamma_{00} = 0, |t^1|, |t^2| \leq \pi\}$ and bound states of the isolated atom remains as before, but the form of the quasistationary bands is changed by the presence of singularities on the discontinuity surfaces $\lambda = |\mathbf{t}|^2$.

When a direct interaction of the nearest neighbors is switched on through nontrivial overlap integrals the lines of the roots $\Delta(\lambda) - \gamma_{11} = 0$ are curved. This leads to a broadening of the corresponding real bands and, perhaps, to overlapping of the gaps due to the resonances.

Thus, as in the case of a three-dimensional crystal, a resonance in the spectrum of the isolated atom leads in the crystal to the appearance of gaps or, at least in the presence of overlapping, to a change in the multiplicity of the spectrum. An important difference of these lower-dimension lattices is the presence of quasistationary bands, which when $k^2 > |\mathbf{t}|^2$ are situated in the cylinder $|t^1|, |t^2| \leq \pi, -\infty < k < \infty$. In physics studies (see, for example, [2]) the quasistationarity of these bands is attributed to the fact that the quasimomentum $\mathbf{t}$ of the waveguide functions that corresponds to them can be obtained by projecting onto the lattice the momentum $k\mathbf{v}$ of the scattered wave having the same energy. One says that a transition between the waveguide state of an electron in the lattice and the corresponding scattered wave is possible.

An interesting question related to the quasistationary bands is their dependence on the resonances of the isolated atom. This question will be discussed in a following publication.

4. Finally, we calculate the S matrices corresponding to the considered crystals of "incomplete dimension" in three-dimensional space. In accordance with Proposition 2 of the present paper, the scattered waves can be expressed in terms of the lattice sums γ_s, s = 1, 2, as follows:

$$\Psi_s^{\Gamma, B}(\mathbf{x}, \mathbf{v}) = e^{-ik\langle \mathbf{x}, \mathbf{v}\rangle} + \rho_{\Gamma, B}((k+i0)\mathbf{v}) \sum_{\mathbf{n}\in\mathbb{Z}^s} \frac{e^{ik|\mathbf{x}-\mathbf{n}|}}{4\pi|\mathbf{x}-\mathbf{n}|} e^{-ik\langle \mathbf{v}, \mathbf{n}\rangle}.$$

We use the formula given in [4] to calculate the asymptotic behavior of the sum $\sum_{\mathbf{n}\in\mathbb{Z}^s} \frac{e^{ik|\mathbf{x}-\mathbf{n}|}}{|\mathbf{x}-\mathbf{n}|}$ $e^{-ik\langle \mathbf{v}, \mathbf{n}\rangle}$ as $|\mathbf{x}|\to\infty$:

$$\sum_{\mathbf{n}\in\mathbb{Z}^s} \frac{e^{ik|\mathbf{x}-\mathbf{n}|}}{4\pi|\mathbf{x}-\mathbf{n}|} e^{-ik\langle \mathbf{v}, \mathbf{n}\rangle} \underset{\mathbf{x}\to\boldsymbol{\omega}\cdot\infty}{\approx} \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|} \sum_{\mathbf{n}\in\mathbb{Z}^s} \exp(ik\langle \mathbf{n}, \boldsymbol{\omega}+\mathbf{v}\rangle) = \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|} \sum_{\mathbf{n}\in\mathbb{Z}^s} \delta(2\pi\mathbf{n} + k(\boldsymbol{\omega}+\mathbf{v})).$$

This gives for the scattering amplitudes the formulas

$$f^{\Gamma, B}(\boldsymbol{\omega}, \mathbf{v}) = \rho_{\Gamma, B}(k+i0, \boldsymbol{\tau}) \sum_{\mathbf{n}\in\mathbb{Z}^s} \delta(2\pi\mathbf{n} + k(\boldsymbol{\omega}+\mathbf{v})),$$

where $\boldsymbol{\tau}$ is the projection of the vector $k\mathbf{v}$, which determines the energy and direction of incidence of the plane wave, onto the plane (line) of the lattice. Because of the presence of the δ functions, the scattering amplitude is nonzero only for directions $\boldsymbol{\omega}, \mathbf{v}$ whose projections P_ω, P_v onto the plane (line) of the lattice are connected by the Laue conditions: $k(P_\omega - P_v) = 2\pi\mathbf{n}$, where $\mathbf{n}$ is an integral vector of the lattice. It follows from the explicit form of the function that in the Laue directions at energies near sharp resonances of the isolated atom sharp resonances will also be observed.

5. We now compare the results obtained in our study with the investigations of other authors. A mathematically rigorous and complete solution to the spectral problem corresponding to scattering by one- and two-dimensional lattices of zero-range potentials was given by Karpeshina [4-7]. Earlier expositions of these problems are contained in [8,9]. These studies described the scattered waves and identified the waveguide band responsible for propagation of electron perturbations along the chain (respectively, lattice). In our work, we have given a rigorous version of a considerably fuller model, which, in particular, contains all the details in the earlier studies and also some new ones. Thus, in our model there may be one or several waveguide bands. In addition, we have the resonance bands whose existence was noted earlier in physics studies (see [2]). Finally, in our model it can be clearly seen that the resonances of the isolated atom lead to diverse spectral phenomena of the type of the occurrence of forbidden bands. In the ordinary model of zero-range potentials, these last two effects could be observed only in the case of a complicated geometry of the individual clusters that form the lattice. In the case of simple cubic point lattices, these effects do not occur.

The appearance in the spectrum of a gap due to a sharp resonance is evidently not related to the regularity of the lattice and can also be observed in the general case of nonperiodic (even random) potentials. Physical arguments for this assertion are put forward in [10].

We thank the referee for drawing our attention to the paper [9].

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ON DISCRETENESS OF THE SPECTRUM OF SOME OPERATOR SHEAVES ASSOCIATED WITH A PERIODIC SCHRÖDINGER EQUATION

V. V. Dyakin and S. I. Petrukhnovskii

Three-dimensional periodic Schrödinger operators with potentials that are square integrable on the unit cell (single-electron model of a crystal) are considered. A description is given of the class of rational curves that do not have more than a finite number of common points with any isoenergy surface (in particular, the Fermi surface) of an arbitrary operator of the considered form. A consequence of a theorem proved in the paper is the absence on the isoenergy surfaces of elements of planes, cones, and cylinders with straight generators, and all possible paraboloids and hyperboloids. Another interesting consequence is the following assertion: The topological dimension of an isoenergy manifold does not exceed two, which justifies the use of the word "surface." The results generalize the assertion of Thomas's theorem on the absence on isoenergy surfaces of straight edges.

1. In quantum solid-state theory an important role is played by the single-electron model of a crystal [1,2], in which the ensemble of electrons, which interact with one another and the ion core, is replaced by an ideal gas of quasiparticles in the field of a periodic potential. Such a model leads to the study of a family of eigenvalue problems for "Bloch" Hamiltonians [3] with periodic boundary conditions on the unit cell Ω (the periodicity cell of the potential):

$$(-\Delta-2ik\nabla+k^2+V(x))u(x,k)=\lambda(k)u(x,k), \tag{1.1}$$

where the potential V(x) is a real function in $L_2(\Omega)$, and the wave vector k belongs to the Brillouin zone Ω_B that corresponds to the cell Ω. In the present paper, to be definite, we consider the case $\Omega = [0, 2\pi]^3 \subset R^3$; the corresponding Brillouin zone is $\Omega_B = [0, 1]^3$; the results can be extended to the case of any periodicity in R^3.

For this problem we have the following propositions [1,3,4].

THEOREM 1. For every fixed k, the operator T(k) determined by the differential expression

$$T(k)\equiv-\Delta-2ik\nabla+k^2+V(x)$$

with domain of definition $W_2^2(\Omega)$ is self-adjoint, bounded below, and possesses a compact resolvent in $L_2(\Omega)$.

Here and below, we denote by $W_2^2(\Omega)$ the Sobolev space of functions periodic on Ω and possessing generalized partial derivatives to the second order inclusively that belong to $L_2(\Omega)$.

COROLLARY 1. The spectrum $\Sigma(T(k))$ of the operator T(k) for any fixed k is discrete and has finite multiplicity with an accumulation point at infinity, i.e., the eigenvalues

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Institute of Metal Physics, Ural Scientific Center of the USSR Academy of Sciences.
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