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# Interaction of a free wave with a semicrystal.

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The Schrödinger operator with a semiperiodic potential describes a motion of a particle in a solid body and the influence of a surface on this motion. It is known that there are three branches of the spectrum corresponding to a semiperiodic potential. They are: the branch coinciding with the spectrum of the free operator, the branch coinciding with the spectrum of the whole crystal, and the branch, corresponding to surface states.

We consider a free wave $\exp(i(\mathbf{k},x))$ which is incident upon the crystal. Interacting with the semicrystal reflected and refracted waves arouse. We construct asymptotic formulae for them when the momentum $\mathbf{k}$ belongs to a rich set $\chi(k,V,\delta)$ on the sphere $|\mathbf{k}| = k$, $k \to \infty$. It is proved that there is no essential reflection inside the crystal and on the surface when $\mathbf{k} \in \chi(k,V,\delta)$. Hence, the reflected wave is small and the refracted one is close to the incident wave $\exp(i(\mathbf{k},x))$. Constructing more precisely the asymptotic formulae of the reflected wave, we describe the connection of the asymptotic terms with the potential in explicit form. This description enable us to determine the potential from the asymptotic expansion of the reflection coefficients in a high energy region when it is known beforehand that the potential is a trigonometric polynomial.

Thus, we consider the operator

$$H_+ = -\Delta + V_+ \tag{1}$$

in $L_2(R^n)$, $n = 2,3$, where $V_+$ is the operation of multiplication by the potential:

$$V_+(x) = \begin{cases} V(x) & \text{if } x_1 \geq 0; \\ 0 & \text{if } x_1 < 0; \end{cases} \tag{2}$$

$V$ being a periodic potential, a trigonometric polynomial. We suppose its period $a_1$ lies on the axis $x_1$ and is orthogonal with the others, namely with $a_2$ when $n = 2$ and with $a_2$, $a_3$ when $n = 3$. For the sake of simplicity we assume that in the three-dimensional case the periods $a_2$, $a_3$ are orthogonal, however all the results are valid also for the case of non-orthogonal periods. Let $x_{||}$ be the projection of the vector $x$ on the plane $x_1 = 0$, namely, $x_{||} = (x_2, x_3)$ for $n = 3$, $x_{||} = x_2$ for $n = 2$. Let $Q_{||}$ be the elementary cell of the periods in the plane $x_1 = 0$:

$$Q_{||} = [0,a_2) \times [0,a_3), \text{ when } n = 3,$$

$$Q_{\|} = [0, a_2), \text{ when } n = 2.$$

The potential is periodic in the direction(s) $x_{\|}$. Following I. M. Gelfand [1], we consider the family of operators $H_+(t_{\|})$ described by formula (1) and the quasiperiodic boundary condition(s) in the strip $Q$:

$$Q = Q_{\|} \times (-\infty, \infty)$$

For the case of $n = 3$ (and orthogonal periods $a_2$, $a_3$) the quasiperiodic conditions have the form:

$$\begin{aligned} \psi(x + a_2, t_{\|}) &= \exp(it_2 a_2)\psi(x, t_{\|}), \\ \psi(x + a_3, t_{\|}) &= \exp(it_3 a_3)\psi(x, t_{\|}). \end{aligned} \tag{3}$$

and there are similar conditions for the first derivatives with respect to $x_1$. The quasimomentum $t_{\|}$, $t_{\|} = (t_2, t_3)$ parametrizing the conditions varies over the elementary cell of the dual lattice:

$$K_{\|} = [0, 2\pi a_2^{-1}) \times [0, 2\pi a_3^{-1}). \tag{4}$$

In the case of $n = 2$ there is only the first relation of (3) and $t_{\|} = t_2$, $K_{\|} = [0, 2\pi a_2^{-1})$. The spectrum of $H_+$ is the union of the spectra of the operators $H_+(t_{\|})$. The eigenfunctions of $H_+$ are obtained by the quasiperiodic extensions of the eigenfunctions of $H_+(t_{\|})$.

We look for a solution $\Psi \in W_2^2(Q)$ of the equation $H_+\psi = k^2\psi$ in the form:

$$\Psi(\mathbf{k}, x) = \begin{cases} \exp(i(\mathbf{k}, x)) + \Psi_{refl}(\mathbf{k}, x), & x_1 \le 0, \\ \Psi_{refr}(\mathbf{k}, x), & x_1 \ge 0, \end{cases} \tag{5}$$

where $\exp(i(\mathbf{k}, x))$ is an incident wave; $k_1 > 0$, $|\mathbf{k}|^2 = k^2$; $\Psi_{refl}$ is a reflected wave, $\Psi_{refr}$ is a refracted wave. The reflected wave we define as follows. Let a function $\psi_-(k^2 + i\varepsilon, t_{\|}, x)$ satisfy the equation $-\Delta\psi_- = (k^2 + i\varepsilon)\psi_-$ and the quasiperiodic conditions (3) when $x_1 \le 0$ for all $\varepsilon$ in a closed upper neighbourhood of zero ($0 \le \varepsilon \le \varepsilon_0$) and let it depend analytically on $i\varepsilon$ in this region for any fixed $x_1 \le 0$. Let $\psi_-(k^2 + i\varepsilon, t_{\|}, x)$ decay exponentially when $x_1 \to -\infty$ for all $\varepsilon$ with a positive real part. Then the function $\Psi_{refl} = \psi_-(k^2 + i0, t_{\|}, x)$ is called a reflected wave, i.e., we call a function $\Psi_{refl}$ a reflected wave if it can be represented as a $\lim_{\varepsilon \downarrow 0} \psi_-(k^2 + i\varepsilon, t_{\|}, x)$, where $\psi_-(k^2 + i\varepsilon, t_{\|}, x)$ is as described above.

The refracted wave we describe as follows. Let a function $\psi_+(k^2 + i\varepsilon, t_{\|}, x)$ satisfy the equation $(-\Delta + V)\psi_+ = (k^2 + i\varepsilon)\psi_+$ and the quasiperiodic conditions (3) when $x_1 \ge 0$ for all $\varepsilon$ in a closed upper neighbourhood of zero ($0 \le \Re\varepsilon \le \varepsilon_0$) and let it depend analytically on $i\varepsilon$ in this region for any fixed $x_1 \ge 0$. Let $\psi_+(k^2 + i\varepsilon, t_{\|}, x)$ decay exponentially when $x_1 \to \infty$ for all $\varepsilon$ with a positive real part. Then the function $\Psi_{refr} = \psi_+(k^2 + i0, t_{\|}, x)$ is called a refracted wave, i.e., we call a function $\Psi_{refr}$ a refracted wave if it can be represented as a $\lim_{\varepsilon \downarrow 0} \psi_+(k^2 + i\varepsilon, t_{\|}, x)$, where $\psi_+(k^2 + i\varepsilon, t_{\|}, x)$ is as described above. These definitions mean that the reflected and refracted waves decay simultaneously under a dissipation,[1] while the incident wave does not. The incident wave $\exp(i(\mathbf{k},x))$ satisfies the quasiperiodic conditions (3) with $t_{||}$:

$$t_i = k_i - 2\pi a_i^{-1}[k_i a_i/2\pi], \tag{6}$$

where $i = 2,3$ when $n = 3$ and $i = 2$ when $n = 2$. Naturally, we look for reflected and refracted waves satisfying the quasiperiodic conditions with the same $t_{||}$. Suppose $\mathbf{k}$ is such that $t = \mathbf{k}$ belongs to the nonsingular set for the periodic potential $V$ [2],[3]. Then, a wave close to $\exp(i(\mathbf{k},x))$ can propagate inside the crystal. Therefore, the continuity conditions on the surface can be satisfied by these waves with an accuracy to $o(1)$ $(k \to \infty)$, the reflected wave being equal to zero. The question arises: is this approximate solution close to the accurate one (5), satisfying the continuity conditions. To answer this question, first of all we clear out whether reflected and refracted waves are defined uniquely. In fact, suppose the equation $H_+\Psi = k^2\Psi$ has a smooth solution $\Psi_{surf}$ which is a reflected wave for $x_1 \leq 0$ and a refracted wave for $x_1 \geq 0$. This solution is called a surface state. Obviously, in this case the reflected and refracted waves in (5) are not uniquely determined. However, the nondecaying component of the reflected and refracted waves are uniquely determined, because surface states exponentially decay as $x_1 \to \pm\infty$. Note, that the operator $(H_+(k_{||}) - z)^{-1}$ has a pole at the point $z = k^2$ in the case of a surface state. In the two and three-dimensional situations surface states can exist in a high energy region, while in the one-dimensional situation they can exist only for sufficiently low energies.

It looks that the surface of the crystal can essentially influence the nondecaying part of the reflected wave even when there is no surface state. This takes place when there exists a solution of the equation $H_+\psi = k^2\psi$, which can be approximated with a good accuracy by a reflected and refracted wave in the sense that the error in the continuity conditions on the surface is small. We call such a solution a quasisurface state. A quasisurface state can influence strongly the asymptotics of the reflected and refracted waves. Unlike the surface state it can also influence the nondecaying component of the reflected wave. It is easy to see that all the points close to surface states are quasisurface states. In the one-dimensional situation there are only these trivial cases: there are no quasisurface states not being in a vicinity of surface states. The similar situation is in the case of separable variables in the two and three-dimensional spaces. However, it seems that quasisurface states can exist separately from surface states in the case of nonseparated variables. We suppose that there corresponds a pole of the resolvent on the non-physical sheet in a vicinity of the point $z = k^2$ to such states.

We are not going to describe surface and quasisurface states here. Our aim is to describe a nonsingular set $\chi(k, V, \delta)$ of $\mathbf{k}$ on the sphere $S_k = \{|\mathbf{k}| = k\}$ for which the influence of the surface and quasisurface states is weak, i.e., the reflected and refracted waves have regular asymptotics determined by a segment of the perturbation series for the resolvent. We can show that it takes place

[1] Of course, the relations $k_1 > 0$, $\varepsilon > 0$ are not fundamental. It is important only that $k_1$, $\varepsilon$ have the same sign. The case $k_1 < 0$, $\varepsilon < 0$ is complexly conjugate for the case $k_1 > 0$, $\varepsilon > 0$.

when there are no surface and quasisurface states with quasimomentum $k_{||}$ in a vicinity of the point $k^2$. ¿From the geometrical point of view the situation in the two-dimensional case is relatively simple. In order to exclude all the surface and quasisurface states it suffices to delete from $S_k$ only the nonsingular set for the periodic part of the potential $V_+$ [2]. The situation becomes more complicated in the three-dimensional case. To exclude the surface and quasisurface states in the three-dimensional situation one has to delete not only the singular set of the periodic part of $V_+$ [3], but also some additional set corresponding namely to surface and quasisurface states. We prove that the reflected wave is asymptotically small and the refracted wave is close to the incident wave when $\mathbf{k}$ belongs to the nonsingular set for the semicrystal $\chi(k,V,\delta)$. However, this weak asymptotic is not able to give an information about the potential. To obtain the information about the potential we describe the reflected and refracted waves more precisely. First we consider the functions satisfying the Helmholtz equation $-\Delta\psi = k^2\psi$ and the quasiperiodic conditions in $||$-directions with the quasimomentum $k_{||}$. It is clear that this set contains the functions

$$\Psi^0_{\pm}(k^2, k_{||}+p_{q_{||}}(0), x) = \exp(i(k_{||}+p_{q_{||}}(0), x_{||}) \pm i\sqrt{k^2-|k_{||}+p_{q_{||}}(0)|^2}x_1),$$

$$q_{||} \in Z^{(n-1)}, \tag{7}$$

where $Im\sqrt{\ } > 0$, $p_{q_{||}}(0) \in R^{n-1}$,

$$p_{q_{||}}(0) = (\frac{2\pi q_2}{a_2}, \frac{2\pi q_3}{a_3})$$

in the three-dimensional situation and

$$p_{q_{||}}(0) = \frac{2\pi q_2}{a_2}$$

in the two-dimensional case. Obviously, the function $\Psi^0_+(k^2, k_{||}+p_{q_{||}}(0), x)$ depends analytically on $k^2$ in the complex plane with the cut along the semiaxis $k^2 < |k_{||}+p_{q_{||}}(0)|^2$. We assume $k_1$ to be positive for the incident wave. Note that

$$\exp(i(\mathbf{k}, x)) = \Psi^0_+(k^2, k_{||}, x). \tag{8}$$

Considering that $\Im\sqrt{k^2+i\varepsilon-|k_{||}|^2} > 0$, when $\varepsilon > 0$, we see that the functions $\Psi^0_+(k^2+i\varepsilon, k_{||}+p_{q_{||}}(0), x)$ increase exponentially when $x_1 \to -\infty$ and decays exponentially when $x_1 \to +\infty$. Therefore, they are not reflected waves. Conversely, the functions $\Psi^0_-(k^2+i\varepsilon, k_{||}+p_{q_{||}}(0), x)$ increase when $x_1 \to +\infty$ and decays when $x_1 \to -\infty$. Therefore they are reflected waves. Thus, we look for the reflected wave as a linear combination of the $\Psi^-_0(k^2, k_{||}+p_{q_{||}}(0), x)$:

$$\Psi_{refl}(k^2, k_{||}, x) = \sum_{q \in Z^{n-1}} \alpha_{q_{||}} \Psi^-_0(k^2, k_{||}+p_{q_{||}}(0), x), \tag{9}$$

where $\alpha_{q_{||}}$ are the reflection coefficients. One has to choose the reflection and refraction waves in such a way that the continuity conditions at the plane $x_1 = 0$

for the corresponding eigenfunctions and its derivative with respect to $x_1$ are fulfilled.

Let $t$ belong to the nonsingular set for the periodic potential $V$. Then the wave close to $\exp(i(\mathbf{k},x))$ can propagate in the crystal [2, 3]. Therefore, the continuity conditions can be satisfied with an accuracy to $O(k)$. Suppose there exists not only a wave close to $\exp(i(\mathbf{k},x)) = \Psi_0^+(k^2, k_{||}, x)$, but also there exist waves close to $\Psi_0^+(k^2, k_{||}+p_{q_{||}}(0), x)$ when $|q_{||}| < k^{9\delta}$. In this case we can satisfy the continuity conditions with an accuracy to $O(k^{-k^{2\delta}R_0^{-1}})$. Then we must take care of the small error in the continuity conditions not to cause a considerable errow in the reflection coefficients. That is, one has to eliminate the situation when the incident wave interacts with the surface and quasisurface states. We construct the nonsingular set $\chi(k,V,\delta)$, which satisfies all these conditions.

First, in the two-dimensional case we show that the wave $\Psi(\mathbf{k},x)$, which propagates inside the crystal and close to the free wave $\exp(i(\mathbf{k},x))$, admits the following asymptotic expansion on the surface of the crystal:

$$\Psi(\mathbf{k},x)\mid_{x_1=0}= \exp(i(\mathbf{k},x))((2ik_1)^{-1}+\sum_{j_{||}\in Z^{n-1}} \exp(i(\mathbf{p}_{j_{||}}(0),x))\sum_{r=1}^{\infty}(A_r)_{j_{||},0}, \quad (10)$$

$$(A_r)_{j_{||},0} = \frac{(-1)^r}{2\pi i}\oint_{C(k_{||})}\sum_{j_1\in Z}[((H_0(\tau)-z)^{-1}V)^r(H_0(\tau)-z)^{-1}]_{j,0}d\tau_1, \quad (11)$$

where $C(k_{||})$ is the circle of radius $k^{-2-2\delta}$ around the point $\tau_1 = \sqrt{k^2-k_{||}^2}$. The derivative of the eigenfunction can be determined analogously:

$$\partial\Psi(\mathbf{k},x)\partial x_1\mid_{x_1=0}=$$

$$\exp(i(\mathbf{k},x))(1/2+\sum_{j_{||}\in Z^{n-1}} \exp(i(\mathbf{p}_{j_{||}}(0),x))\sum_{r=1}^{\infty}(B_r)_{j_{||}+m_{||},m_{||}}, \quad (12)$$

$$(B_r)_{j_{||}+m_{||},m_{||}} = \quad (13)$$

$$\frac{(-1)^r}{2\pi i a_1}\oint_{C(m_{||})}\sum_{j_1\in Z}(\tau_1+2\pi j_1+2\pi m_1)[((H_0(\tau)-z)^{-1}V)^r(H_0(\tau)-z)^{-1}]_{j+m,m}d\tau_1.$$

In the case of $n=3$ a similar expansion is valid (we have to replace $V$ by $W$ and $H_0$ by $\hat{H}$ in the formulae for $A_r$ and $B_r$ [3]).

If $t$ belongs to the nonsingular set $\chi(k,\delta,V)$, the expansions (11) and (13) are valid not only for $\Psi(\mathbf{k},x)$ but also for $\Psi(k_{q_{||}},x), q_{||}\in Z^{n-1}, \mid q_{||}\mid< k^{9\delta}$,

$$k_{q_{||}} = (k_{||}+p_{q_{||}}(0), (k^2- \mid k_{||}+p_{q_{||}}(0)\mid^2)^{1/2}). \quad (14)$$

Therefore one can introduce the matrices $A_{jr}$ and $B_{jr}$, where $\mid j\mid\le k^{\delta}, \mid r\mid\le k^{\delta}$. Let us consider these matrices as infinite ones, assuming $A_{jm}$ and $B_{jm}$ to be zero for $\mid j\mid$ or $\mid r\mid$ being more than $k^{\delta}$.

Let us introduce the diagonal matrix $K$:

$$K_{q_{||}q_{||}} = (k^2- \mid k_{||}+p_{q_{||}}(0)\mid^2)^{1/2}. \quad (15)$$

This matrix is invertable when $t \in \chi(k,\delta,V)$. Let

$$A = \sum_{r=1}^{N(k)} A_r, B = \sum_{r=1}^{N(k)} B_r, N(k) = [k^{9\delta} R_0^{-1}], \tag{16}$$

$$C = KA + B = \sum_{r=1}^{N(k)} C_r.$$

Now we formulate the asymptotic expansion theorem for the reflected wave coefficients.

**Theorem 1** . *If $t$ is in the $(k^{-n+1-2\delta})$-neighbourhood of $\chi_5(k,\delta,V)$ for a sufficiently large $k, k > k_0(V,\delta)$, then the following asymptotic expansion for $\alpha_{m_\| + j_\|, m_\| + q_\|}$ is valid:*

$$\alpha_{m_\|+j_\|,m_\|+q_\|} = \alpha^0_{m_\|+j_\|,m_\|+q_\|} + O(k^{-k^{2\delta} R_0^{-1}}), \tag{17}$$

$$\alpha^0_{m_\|+j_\|,m_\|+q_\|} = (2K)^{-1}(C - 2KA)(I + C)^{-1}(2K). \tag{18}$$

*The asymptotic expansion (17) is valid for $A, C$, since the following estimates for $A$ and $C$ are fulfilled:*

$$\|KA_r\|_1 < k^{-\zeta r},$$

$$\|C_r\| < K^{-\zeta r}, \ \zeta = \zeta(n,\delta) > 0. \tag{19}$$

We can also obtain the refraction coefficients. The asymptotic formulae for both the reflection and refraction coefficients are infinitely differentiable with respect to $k$.

The main aim of Theorem 1 is just to justify the asymptotic expansion. Using this theorem, we obtain a simpler asymptotic formula for the reflection coefficients. To describe it let us introduce some new notations. Let $v_{q_\|}(x_1)$ be the Fourier coefficients of $V$ with respect to $x_\|$:

$$v_{q_\|} = w \int V(x) \exp(i(p_{q_\|}(0), x_\|)) dx_\|,$$

$$w = a_2^{-1} \text{ when } n = 2,$$

$$w = a_2^{-1} a_3^{-1} \text{ when } n = 3.$$

Let $V^{(r)}(0)$ be the vector whose elements are the derivatives of the functions $v_{q_\|}(x_1)$ of $r$ order with respect to $x_1$ at the point $x_1 = 0$:

$$V^{(r)}(0)_{q_\|} = (\partial^r v_{q_\|} / \partial x_1)(0).$$

**Theorem 2** . *If $t$ is in the $(k^{-n+1-2\delta})$-neighbourhood of $\chi(k,\delta,V)$ for sufficiently large $k, k > k_0(V,\delta)$, then the following asymptotic expansion for $\alpha_{m_\|+j_\|,m_\|+q_\|}$, $| q_\| | < k^\delta$ is valid:*

$$\alpha_{m_\|+j_\|,m_\|+q_\|} = \alpha^0_{m_\|+j_\|,m_\|+q_\|} + O(k^{-k^{2\delta} R_0^{-1}}), \tag{20}$$

$$\alpha^0_{m_\parallel+j_\parallel,m_\parallel+q_\parallel} = (2K_{j_\parallel j_\parallel})^{-1}\sum_{r=0}^{\infty}(\Phi_r)_{m_\parallel+j_\parallel,m_\parallel+q_\parallel}(K_{j_\parallel j_\parallel}+K_{q_\parallel q_\parallel})^{-r-1}, \qquad (21)$$

*where* $K_{j_\parallel j_\parallel}$ *and* $K_{q_\parallel q_\parallel}$ *are the elements of the matrix* $K$ *(see (15)),* $K_{q_\parallel q_\parallel} \approx k$, $\Phi_r$ *are given by the formula:*

$$(\Phi_r)_{m_\parallel+j_\parallel,m_\parallel+q_\parallel} = \qquad (22)$$

$$i^r V^{(r)}(0)_{j_\parallel-q_\parallel} + (\varphi_r(V(0),...,V^{(r-1)}(0))_{m_\parallel+j_\parallel,m_\parallel+q_\parallel},$$

*where* $\varphi$ *is a polynomial matrix-function of* $V(0),...,V^{(r-1)}(0)$, $\varphi_0 = 0, \varphi_r = O(1)$, *when* $k \to \infty$.

It is easy to see that

$$\varphi_r = \tilde{\varphi}_r(\Phi_0,...,\Phi_{r-1}).$$

Furthermore, one can obtain the vectors $V^{(r)}(0)$ by the recursive procedure:

$$V(0)_{j_\parallel} = \lim_{k\to\infty}(\alpha_{m_\parallel+j_\parallel,m_\parallel}2K_{j_\parallel j_\parallel}(K_{j_\parallel j_\parallel}+K_{q_\parallel q_\parallel}), \qquad (23)$$

$$V^{(1)}(0)_{j_\parallel} = \qquad (24)$$

$$-i\lim_{k\to\infty}(\alpha_{m_\parallel+j_\parallel,m_\parallel}2(K_{j_\parallel j_\parallel}(K_{j_\parallel j_\parallel}+K_{q_\parallel q_\parallel})^2 - V(0)_{j_\parallel}(K_{j_\parallel j_\parallel}+K_{q_\parallel q_\parallel}) - \phi_1(V(0)),$$

and so on. We use these relations for the solution of the inverse problem.

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