Eigenfunction expansion of a Schrödinger operator with a complex potential

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A localization is presented of the spectrum of the operator $L = -(\partial^2/\partial x^2) + u(x)$ with a complex periodic potential $u(x)$. Formulas are presented for the expansion of functions that are summable over $(-\infty, \infty)$ in eigenfunctions of the operator and of the Parseval equation.

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1. Within the framework of the potential model of scattering with energy absorption, the potential $u(x)$ is complex, and in a medium with a crystal structure it is also periodic. This explains the need for solving the problem of eigenfunction expansion of the Schrödinger operator $L_u = -(\partial^2/\partial x^2) + u(x)$ with a complex periodic potential $u(x) = u(x+\tau)$.

As is well known, the spectrum of an operator with a continuous periodic real potential consists of an infinite half-line $E \geq E_0$, from which an infinite or finite number of forbidden intervals (lacunae) have been removed.

Let E be a point of the continuous spectrum and let $\phi_{1,2}(x;E)$ be a certain fundamental system of solutions of the equation $(L-E)\phi = 0$, and let $T(E)$ be a matrix defined by

$$T(E) = \begin{pmatrix} a_{11} a_{12} \\ a_{21} a_{22} \end{pmatrix}, \quad \phi_i(x+\tau) = a_{i1}\phi_1(x) + a_{i2}\phi_2(x), \quad i = 1,2 \tag{1}$$

The trace of $T(E)$ and the eigenvalues $\rho_{1,2}(E)$ do not depend on the choice of the basis $\phi_{1,2}(x;E)$. $F(E) = (1/2)\mathrm{Tr}\, T(E)$ is an entire function and behaves asymptotically like $\cos \tau\sqrt{E_0}$. Since $\det T(E) = 1$, we have

$$\rho_{1,2}(E) = F(E) \pm i\sqrt{1 - F^2(E)}. \tag{2}$$

The fact that the point E belongs to the continuous spectrum means that all the solutions of the equation $(L-E)\phi = 0$ are bounded along the entire axis. This is equivalent to the equality $|\rho_{1,2}(E)| = 1$. Since $\rho_1\rho_2 = 1$, this yields $\rho_{1,2}(E) = \exp[ip(E)\tau]$, where $\rho(E)$ is a real quasimomentum. Comparison with (2) yields

$$F(E) = \cos\tau\, p(E), \qquad \mathrm{Im}F(E), \qquad |F(E)| \leq 1,$$
$$\tau p(E) = i\ln[F(E) - i\sqrt{1 - F^2(E)}] \tag{3}$$

(the sign of the root is such that $p(E) \sim i\ln 2F(E)$ as $E \to -\infty$. The derivation of (4) does not require that the potential $u(x)$ be real, i.e., the following general statement has been proved:

The spectrum of the operator $L = -(\partial^2 u/\partial_x^2) + u(x)$ with real or complex potential coincides with the set

$$\mu(E: \mathrm{Im}\,\mathrm{Sp}\, T(E) = 0, \quad \mathrm{Sp}\, T(E) \leq 2). \tag{4}$$

A rough asymptotic estimate of $\mathrm{Tr}\, T(E)$ does not depend on whether the potential is real, so that the structure of the spectrum μ is asymptotically the same as in the case of a real potential. It is important that the plane with the spectrum removed remains connected, since μ cannot contain closed curves. Sets of this type were investigated in detail in[1].

2. Knowledge of the spectrum makes it possible to obtain the following theorem concerning eigenfunction expansions.

Let the function $f(x)$ belong to $L(-\infty,\infty)$ and have a bounded variation in the vicinity of the point x; then

$$f(x) = \frac{1}{4\pi} \int_\mu \frac{\phi(E)\,dE}{\sqrt{1 - F^2(E)}} [\psi_1(x;E)h_2(E) + \psi_2(x;E)h_1(E)]dE. \tag{5}$$

Here $\psi_i(x;E)$ is the Bloch function of the operator L, and

$$h_i(E) = \int_{-\infty}^{\infty} \psi_i(x;E) f(x)\,dx, \quad i = 1, 2. \tag{6}$$

We have $\phi(E) = \phi(\tau;E)$, where $\phi(x;E)$ is the solution of the equation $(L-E)\phi = 0$ with initial conditions $\phi(0;E) = 0$ and $\phi'(0;E) = 1$. The integration in (5) is over μ as along a cut, i.e., on both edges of each arc contained in μ. The function $\sqrt{1 - F^2(E)}$ is unique in the plane with the removed spectrum μ, and the sign of the root is determined by the condition $\sqrt{1 - F^2(E)} \sim -iF(E)$ as $E \to -\infty$.

For a real potential, formula (5) is a transformation of formula (21.6.3) of[2]. The proof given in[2] is based entirely on the asymptotic forms of $F(E)$ and $\psi_{1,2}(x;E)$, which do not change in the case of a complex potential; this proves the representation (5).

From (5) we arrive directly at the Parseval equation equation

$$\int_{-\infty}^{\infty} f^2(x)\,dx = \frac{1}{2\pi} \int_\mu \frac{\phi(E)\,dE}{\sqrt{1 - F^2(E)}} h_1(E) h_2(E). \tag{7}$$

We transform formulas (5)—(7) to a form close to the Fourier transformation. The spectrum μ lies on one branch of the curve $\mathrm{Im}F(E) = 0$, and E_0 is its starting point. We draw from the point E_0 a cut along this curve. The function $p(E)$ (see (3)) maps conformally the plane E with the cut onto the half-plane $\mathrm{Im}\, p > 0$, with vertical final cuts that emerge from points that are multiples of π. The transform of the spectrum μ fills the entire real axis, and the spectrum points $E_\pm$ on opposite edges correspond to the points $\pm p$. As is well known,

$$\psi_{1,2}(x;E) = \exp(\pm ip(E)x)\chi_{1,2}(x;E), \quad \chi(x+r;E) = \chi(x;E). \tag{8}$$

It is easy to verify that $\psi_{1,2}(x;E)$ in (8) are the values of one and the same function $\psi(x,E)$, which is analytic in E, on opposite edges of the cut. The same holds for $\chi_{1,2}(x;E)$. We express E in terms of p ($E=E(p)$). We denote by $\hat{\psi}(x;p)$ and $\hat{\chi}(x;p)$ the functions $\hat{\psi}(x;E)$ and $\hat{\chi}(x;E)$ expressed in terms of p. In terms of the variable p, formulas (5)—(7) become

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dp \frac{\phi[E(p)]}{F'[E(p)]} e^{ipx}\hat{\chi}(x;p)\tilde{f}(-p), \tag{9}$$

$$\tilde{f}(p) = \int_{-\infty}^{+\infty} e^{ixp}\hat{\chi}(x;p)f(x)\,dx, \tag{10}$$

$$\int f^2(x)\,dx = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dp \frac{\phi[E(p)]}{F'[E(p)]}\tilde{f}(-p)\tilde{f}(p) \tag{11}$$

$\phi(E)/F'(E)$ and $\hat{\chi}(x;p)$ tend to unity as $p \to \pm\infty$. These formulas are useful also in the case of a real potential.

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