Quantum physics, Department of Physics, 6th semester.

Lesson №7. ***One-dimensional movement in a field of piecewise continuous potentials(continuation). Schrodinger's equation in momentum representation. Transfer-matrix: calculating of transmission coefficient, energy spectrum of periodic potentials.***

1. Hamiltonian in momentum representation for one-dimensional movement of the particle in stationary external field has the form

$$\hat{H} = \hat{T} + \hat{U} = \frac{p^2}{2m} + U\left(i\hbar\frac{\partial}{\partial p}\right), \quad p_x \equiv p.$$

Thus, in p-representation operator of kinetic energy $\hat{T} = \frac{\hat{p}^2}{2m} = \frac{p^2}{2m}$ is operator of multiplication, operator of potential energy $\hat{U}$ is an integral operator with kernel $U(p, p')$ which equals to

$$U(p, p') = U(p - p'), \quad U(p - p') = \frac{1}{2\pi\hbar}\int U(x) e^{\left\{-\frac{i(p-p')x}{\hbar}\right\}} dx.$$

Consequently, one-dimensional Schrodinger equation in p-representation has the form

$$\frac{p^2}{2m}\Phi(p) + \int_{-\infty}^{\infty} U(p - p')\Phi(p')dp' = E\Phi(p),$$

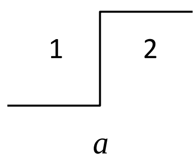
where $C(p)$ is a wave function in p-representation.

Task 1. Analyze a solution of the energy levels problem $(E < 0)$ for the particle in a δ-well $U(x) = -\alpha\delta(x)$ using p-representation.

2. *Transfer-matrix*. Transfer-matrix method is convenient to use for one-dimensional problems with piecewise continuous potentials solving, if potential energy has translation symmetry everywhere, except finite region on real axis.

2.1. Constraint matrix of local solutions.

Let us introduce a constraint matrix of local solutions, which connect solutions of stationary Schrodinger equation in two related areas 1 and 2, if potential has a jump in potential energy at the border of these two areas.



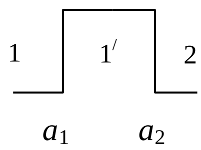
$$\psi_1 = A_1\varphi_1^{(1)} + B_1\varphi_2^{(1)};$$
$$\psi_2 = A_2\varphi_1^{(2)} + B_2\varphi_2^{(2)}.$$

4 coefficients here are connected with two conditions:

$$\psi_1(a) = \psi_2(a);$$
$$\psi_1'(a) = \psi_2'(a).$$

This connection can be written in matrix form $\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{T}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$, where $\hat{T} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}$ – constraint matrix of two local solutions.

2.3 Transfer-matrix



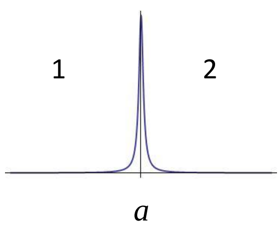
$$\psi_1 = A_1\varphi_1^{(1)} + B_1\varphi_2^{(1)};$$
$$\psi_{1'} = A_{1'}\tilde{\varphi}_1^{(1)} + B_{1'}\tilde{\varphi}_2^{(1)};$$
$$\psi_2 = A_2\varphi_1^{(2)} + B_2\varphi_2^{(2)};$$

Boundary conditions for rectangular barrier (rectangular well) are

$$\psi_1(a_1) = \psi_{1'}(a_1); \quad \psi_1'(a_1) = \psi_{1'}'(a_1);$$
$$\psi_{1'}(a_2) = \psi_2(a_2); \quad \psi_{1'}'(a_2) = \psi_2'(a_2);$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{\hat{T}}_1\begin{pmatrix} A_{1'} \\ B_{1'} \end{pmatrix}; \quad \begin{pmatrix} A_{1'} \\ B_{1'} \end{pmatrix} = \hat{\hat{T}}_{1'}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}; \quad \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{\hat{T}}_1 \cdot \hat{\hat{T}}_{1'}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \hat{T}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}; \quad \hat{T} = \hat{\hat{T}}_1 \cdot \hat{\hat{T}}_{1'}.$$

Boundary conditions for delta-potential $U(x) = \alpha\delta(x-a)$ are



$$\psi_2(a+0) = \psi_1(a-0);$$
$$\psi_2'(a+0) - \psi_1'(a-0) = \frac{2m\alpha}{\hbar^2}\psi(a).$$

The choice of local solutions should be such, that $\mathrm{Det}\hat{T} = 1$.

2.4 How to calculate the transmission coefficient *D*?

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} t_{11}A_2 & t_{12}B_2 \\ t_{21}A_2 & t_{22}B_2 \end{pmatrix};$$

If $B_2 = 0$ (there is no flow of particles from the right to the left), then

$$D = \frac{\left|\vec{j}_{transmitted}\right|}{\left|\vec{j}_{incidental}\right|} = \frac{|A_2|^2}{|A_1|^2} = \frac{1}{|t_{11}|^2}.$$

Task 2. Find the transmission coefficient of the delta-barrier $U(x) = \alpha\delta(x)$ using transfer-matrix method.

2.5. Periodic potential of N same "jumps" with periodic boundary conditions.

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{T}^N \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix}, \quad A_{N+1} = A_1, B_{N+1} = B_1, \Rightarrow, \quad \hat{T}^N = \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$\begin{pmatrix} t_{11} - \lambda & t_{12} \\ t_{21} & t_{22} - \lambda \end{pmatrix} = 0, \quad \lambda^2 - Tr\hat{T} \cdot \lambda + Det\hat{T} = 0,$$

$$Tr\hat{T} = t_{11} + t_{22} = \lambda_1 + \lambda_2;$$

$$\mathrm{Det}\hat{T} = 1, \Rightarrow, \lambda_1 \cdot \lambda_2 = 1, \quad \lambda_1 = \lambda = \exp(i\nu), \lambda_1 = \lambda^* = \exp(-i\nu),$$

$$\lambda^N = \exp(i\nu N) = 1, \quad \nu = \frac{2\pi l}{N}.$$

Dispersion equation

$$\boxed{\mathrm{Tr}\hat{T} = 2\cos\nu}$$

Task 3. Find the dispersion equation for Dirac potential «comb» with $U(x) = \sum_{n=1}^{N} \alpha\delta(x - na)$. (НКК, 1992 № 2.53)

3. Test (~ 20 minutes) – **15 points.**

Hometask НКК 2.48 (using transfer-matrix method), НКК 2.50 (using transfer-matrix method).

НКК – Halitskii E.M., Karnakov B.M., Kohan V.I. Problems in Quantum Physics, 1981

Hr. – Hrechko, Suhakov, Tomasevich, Fedorchenko Collection of theoretical physics problems, 1984