Simple one-dimensional potentials

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Outline

The square well potential and trial wavefunction

We consider the potential

$$V(x) = V_0\left[\Theta(a+x) - \Theta(a-x)\right] = \begin{cases} 0 & (|x| > a), \\ V_0 & (|x| < a). \end{cases}$$

If $V_0 > 0$ then this is the square potential well. Classically it has bound states with all possible energies $0 \le E \le -V_0$, and every positive energy state is unbound. Since $V(x)$ is even under parity, the wavefunctions may also be reduced under parity.

Since bound state wave functions must be normalizable, they have to fall off at infinity. Then, a trial wavefunction of parity λ is

$$\psi(x; E, \lambda) = \begin{cases} A_1 \mathrm{e}^{kx} & (x < -a) \\ A_2\left(\mathrm{e}^{ik'x} + \lambda \mathrm{e}^{-ik'x}\right) & (|x| < a) \\ \lambda A_1 \mathrm{e}^{-kx} & (x > a) \end{cases}$$

where $k = \sqrt{2mE}/\hbar$ and $k' = \sqrt{2m(E+V_0)}/\hbar$.

Dimensionless variables; eigenvalues from matching

Introduce the dimensionless variables

$$r^2 = \frac{2mV_0 a^2}{\hbar^2} \quad \text{and} \quad z = \frac{E}{V_0} = -\left(\frac{ka}{r}\right)^2 = \left(\frac{k'a}{r}\right)^2 - 1.$$

The inverse relations are—

$$ka = r\sqrt{-z} \qquad \text{and} \qquad k'a = r\sqrt{1+z}.$$

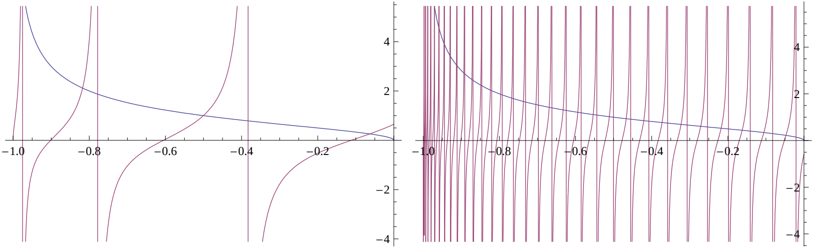
The quantity r parametrizes the potential. Solving the eigenvalue equation amounts to finding z.

Since the matching conditions at $x = \pm a$ give the same results, it is sufficient to examine the conditions at $x = -a$. These give the eigenavalue equation

$$k = \begin{cases} k' \tan k'a & (\lambda = 1) \\ k' \cot k'a & (\lambda = -1), \end{cases} \qquad \text{or} \qquad \left(\frac{-z}{1+z}\right)^{\lambda/2} = \tan r\sqrt{1+z}.$$

Since the eigenvalue equation does not see E, V_0 and a separately, but only the combination z and r, there is a degree of universality about the

Solving for the eigenvalues



The eigenvalues occur whenever the left and right hand sides of the equation cross. The number of eigenvalues increases when r increases (plot on left: $r = 10$, on right: $r = 100$). There are an infinite number of eigenvalues when $r \to \infty$. As r decreases, the levels move up (**why?**) and at a critical r_* one level disappears. As r decreases further, other critical values of r may be reached. For sufficiently small r there may be no bound states.

Universality in the square well potential

When the binding energy is very small, the range of the wavefunction is large. In this case, the detailed shape of the potential cannot be seen by the wavefunction. Thus we expect some level of universality about the problem.
The critical values of r_* are

$$r_* = \begin{cases} n\pi & (\lambda = 1) \\ (n + \frac{1}{2})\pi & (\lambda = -1). \end{cases}$$

In the neigbourhood of these potentials, $r = r_* + \delta$, one finds from the eigenvalue equations that $E \propto \delta^2$. The power is independent of n and λ.
The RMS radius of the wavefunction is

$$\langle x^2 \rangle = 2\int_0^a dx x^2 |\psi(x)|^2 + 2\int_a^\infty dx x^2 |\psi(x)|^2 \simeq \frac{1}{k^2 a^2} \propto (r - r_*)^{-2}$$

where we have used the fact that the second integral dominates when the range is large. (**Check by explicit integration**)

Outline

The transfer matrix for short range potentials

Consider any potential $V(x)$ with a **finite range**, *i.e.*, $V(x) = 0$ for $|x| > a$. Consider a wavefunction which is an incoming plane wave for $x < -a$,

$$\psi(x;k) = \begin{cases} \mathrm{e}^{ikx} & (x < -a) \\ A_k \mathrm{e}^{ikx} + B_k \mathrm{e}^{-ikx}. & (x > a) \end{cases}$$

For any real potential, if $\psi(x)$ is a solution of Schrödinger's equation, then so is $\psi^*(x)$ (**prove**). Hence, the outgoing plane wave on the right, $\psi^*(x;k)$, is also a solution. A general solution is therefore the superposition

$$\psi(x) = \begin{cases} A_1 \mathrm{e}^{ikx} + B_1 \mathrm{e}^{-ikx} & (x < -a) \\ A_2 \mathrm{e}^{ikx} + B_2 \mathrm{e}^{-ikx}. & (x > a) \end{cases}$$

Using the definitions of $\psi(x;k)$ and $\psi^*(x;k)$, one obtains the

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \quad \text{where} \quad M = \begin{pmatrix} A_k & B_k^* \\ B_k & A_k^* \end{pmatrix}.$$

The probability current; reflection and transmission

The probability current, $J = (\psi^* \hat{p} \psi + \psi \hat{p}^\dagger \psi^*)/(2m)$ obeys the continuity equation (**prove**)

$$\frac{dP}{dt} + \frac{dJ}{dx} = 0, \quad \text{where} \quad P = |\psi|^2.$$

For any stationary state, since the time dependence vanishes, J is the same at all points.
For the finite range potentials that we are working with, one finds that $J = (\hbar k)(|A_i|^2 - |B_i|^2)/(2m)$. Using the relation expressed through the marix M above, we find that this gives $|A_k|^2 - |B_k|^2 = 1$, *i.e.*, $\mathrm{Det}\, M = 1$.
The reflection and transmission coefficients are

$$R = \left|\frac{B_k}{A_k}\right|^2 = 1 - T \qquad \text{where} \qquad T = \frac{1}{|A_k|^2}.$$

Clearly $|A_k|^2 \geq 1$. Resonances occur when $R = 0$, *i.e.*, when $|A_k|^2 = 1$.
The barrier is perfectly reflecting when $|A_k|^2 \to \infty$.

The scattering matrix for a short range potential

The scattering matrix connects the incoming waves to the outgoing waves, and hence can be constucted by rearranging the elements of the transfer matrix. A straighforward bit of algebra shows that

$$\begin{pmatrix} A_2 \\ B_1 \end{pmatrix} = S \begin{pmatrix} A_1 \\ B_2 \end{pmatrix}, \quad \text{where} \quad S = \frac{1}{A_k^*} \begin{pmatrix} 1 & B_k^* \\ -B_k & 1 \end{pmatrix}.$$

It is easy to check that S is unitary from the fact that $|A_k|^2 - |B_k|^2 = 1$. In other words, **probability conservation leads to an unitary S-matrix**. At a resonance, $|A_k|^2 = 1$, and hence $|B_k|^2 = 0$. Hence, the resonance condition leads a diagonal S-matrix, *i.e.*, at resonance, an incoming plane waves on the left becomes an outgoing plane wave on the right with a phase shift, and an incoming plane wave on the right becomes an outgoing plane wave on the left with the opposite phase shift. This is exactly the condition that $R = 0$. When $T = 0$, the S-matrix is off-diagonal.

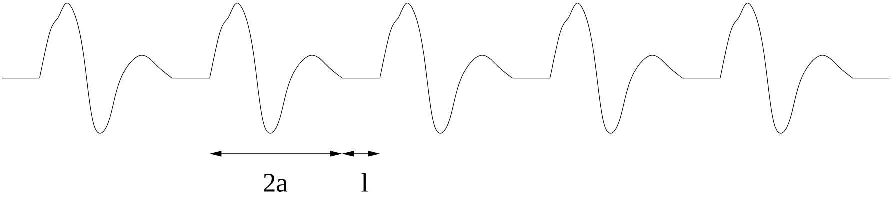
Outline

Bloch's theorem for periodic potentials

If the potential is periodic, $V(x) = V(x + x_0)$, then finite translations $T(x_0)$ commute with the Hamiltonian. Hence finite translations and the Hamiltonian can be diagonalized simultaneously. If $\psi(x)$ is such an eigenfunction, then $T(x_0)\psi(x) = \lambda\psi(x)$. Also, $T^n(x_0)\psi(x) = \lambda^n\psi(x)$. Hence $\lambda = \exp(iKx_0)$ for some choice of K. Hence, any eigenfunction in the period potential has the form $\psi(x + nx_0) = \exp(iKnx_0)\psi(x)$. The last statement is **Bloch's theorem** in one dimension. It is a statement of the fact that finite translations constitute an Abelian group. The value of K depends on the boundary conditions one chooses.

The generalization to arbitrary dimensions is straightforward. If $T(\mathbf{R})$ is a translation by a lattice vector and $T(\mathbf{R}')$ that by another lattice vector, then $T(\mathbf{R})T(\mathbf{R}')\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R} + \mathbf{R}') = T(\mathbf{R}')T(\mathbf{R})\psi(\mathbf{r})$. Hence the group is Abelian in any dimension. Therefore, if the Hamiltonian commutes with these finite translations, then the eigenfunctions of the Hamiltonian must be of the form $\psi(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{K} \cdot \mathbf{R})\psi(\mathbf{r})$.

The step transmission matrix in one dimension



We consider a periodically repeating short ranged potential with range of $2a$ and spacing l between the end of one unit of the potential and the beginning of the next (hence $x_0 = l + 2a$). The wavefunction at any point where the potential vanishes is a superposition of a left moving and a right moving plane wave: $A_i \exp(ikx) + B_i \exp(-ikx)$. A matrix Q connects this to the wavefunction at $x + x_0$. This matrix is

$$Q = \begin{pmatrix} z & 0 \\ 0 & \frac{1}{z} \end{pmatrix} M = \begin{pmatrix} zA_k & zB_k^* \\ \frac{B_k}{z} & \frac{A_k^*}{z} \end{pmatrix}, \quad \text{where} \quad z = \exp(ikl).$$

Eigenvalues of Q and the transmission coefficient

The characteristic equation for Q is

$$\lambda^2 - 2\mathrm{Re} z A_k \lambda + 1 = 0.$$

The solutions have the following form—

1. If $1 \leq \mathrm{Re} z A_k$, then the two eigenvalues are real, and $\lambda_1 \geq 1 \geq \lambda_2$.
2. If $1 > \mathrm{Re} z A_k$, then the two eigenvalues are pure phases: $\lambda_1 = \exp(i\chi)$ and $\lambda_2 = \exp(-i\chi)$.

If $UQU^\dagger$ is diagonal, then

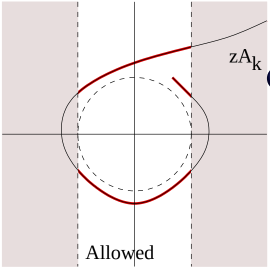
$$Q^N = U^\dagger \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} U.$$

The transmission coefficient through these N copies of the potential is given by the inverse of the 11 component of Q^N. Hence

$$1/T_N = \lambda_1^N \cos^2\theta + \lambda_2^N \sin^2\theta.$$

Here θ depends on the eigenvector $|\lambda_1\rangle$.

Energy bands in one-dimensional periodic potentials



1. If $1 \leq \mathrm{Re} zA_k$, then the two eigenvalues are real, and $\lambda_1 \geq 1 \geq \lambda_2$. Then $\lambda_1^N \gg 1 \gg \lambda_2^N$. As a result, the transmission coefficient drops to zero as $N \to \infty$. These values of zA_k correspond to **band gaps**. In the very special case of $\lambda_1 = \lambda_2 = 1$ the transmission coefficient goes to unity. This is the case of Bragg diffraction.
2. If $1 > \mathrm{Re} zA_k$, then the two eigenvalues are pure phases: $\lambda_1 = \exp(i\chi)$ and $\lambda_2 = \exp(-i\chi)$. In this case $T_N = 1/(\cos^2\theta + \cos 2N\chi \sin^2\theta)$, and this goes to some finite value as $N \to \infty$. Thus, these values of zA_k correspond to **allowed energy bands**.

Outline

References

1. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture are scattered through chapters 2 and 3 of this book. Several of these matters are dealt with in problems.
2. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 3 of this book discusses the material in this lecture.
3. Solid State Physics, by N. W. Ashcroft and N. D. Mermin. Chapter 8 of this book contains a discussion of Bloch's theorem and related topics.
4. An introduction to renormalization for the Schrödinger's equation is given in Section 2 of the paper "How to Renormalize the Schrodinger Equation" by P. Lepage. The paper is available at the URL `http://arxiv.org/abs/nucl-th/9706029`.