Problem Set 6
Physics 386 / Spring 1997
Professor Klaus Schulten

Problem 1: Scattering by an Attractive Well

The following example had been described in class. You are expected to provide the complete derivations.

A particle is scattered by a potential

$$V(x) \;=\; \begin{cases} -V_0 & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \tag{1}$$

where $V_0 > 0$.

(a) Determine the wave function for an incident wave $\exp(ikx)$, $k > 0$.

(b) Determine the transmission coefficient, i.e. the ratio of the transmitted flux to the incident flux, $T(k)$.

(c) Plot the transmission coefficient in a representative range of k-values.

Problem 2 : Model for a Molecular Potential

A simple model for a molecular potential is

$$U(x) \;=\; U_o\delta(x+\frac{a}{2}) \;+\; U_o\delta(x-\frac{a}{2})\,, \quad U_o \;<\; 0 \tag{2}$$

Determine the bound states of the system and discuss the result as a function of a.

Problem 3: Tunneling Through a δ-Barrier and Through a δ-Barrel

Consider the stationary states

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \;+\; U(x) \;-\; \frac{\hbar^2 k^2}{2m} \right] \phi_k(x) \;=\; 0 \tag{3}$$

describing scattering of one-dimensional particles impinging from the left on a potential $U(x) = U_o\delta(x)$, $U_o > 0$.

(a) Show that the derivative of the stationary states $\phi_k(x)$, i.e., $\phi_k'(x)$, have a discontinuity at $x = 0$. Determine the magnitude of the discontinuity, i.e., determine $\lim_{\epsilon \to 0}(\, \phi_k'(\epsilon) - \phi_k'(-\epsilon)\,)$.

(b) Employ the property derived in (a) to deterine the wave function for an incident wave $\exp(ikx)$, $k > 0$.

(c) Determine the transmission coefficient T as a function of U_o and of the energy E of the incoming particles.

(d) Carry out the same calculation (stationary states and transmission, reflection coefficients for particles coming from $x \to -\infty$) for the potential $U(x) = U_o\delta(x) + U_0\delta(x-a)$, $U_o > 0$.

(e) Plot the resulting transmission coefficient T as a function of energy for various U_o

(f) Plot the stationary states determined in (d) for the energy of the first two minima and maxima of $T(E)$.

(g) Discuss the results in (d) and (e), in particular, relate the stationary states corresponding to the maxima of $T(E)$ to the stationary states of a particle in a one-dimensional box of size a.

Problem 4: Bound States of Square Well Potential

A quantum particle of mass m moves in one dimension in the square well potential of width $2a$

$$U(x) = \begin{cases} 0 & |x| > a \\ -U_o & |x| \leq a \end{cases} \tag{4}$$

for $U_o > 0$. Describe the stationary states of such particle for $E < 0$. In your derivation you are asked to formulate in your own terms and in sufficient detail the derivation provided in class, e.g., do not state "as shown in class".

(a) State the wave function in the three regions $x < -a$, $-a < x < a$, $a < x$ and demonstrate that it obeys the time-independent Schrödinger equation. Assume for this purpose symmetric and antisymmetric wavefunctions, i.e., $f(-x) = \pm f(x)$. Explain, in particular, the choice of the wave functions in regions V_I and V_{III} in regard to the property that bound state wave functions need to be square integrable, i.e., $\int_{-\infty}^{\infty} dx\, |\phi_E(x)|^2 < \infty$.

(b) Applying the continuity conditions at $x = \pm a$ show that they require

$$\mathrm{tg}ka = \frac{\sqrt{c^2 - (ka)^2}}{ka} \qquad \text{even wave functions} \tag{5}$$

$$\mathrm{tg}ka = -\frac{ka}{\sqrt{c^2 - (ka)^2}} \qquad \text{odd wave functions} \tag{6}$$

$$k^2 = \frac{2mE}{\hbar^2} + \frac{2mU_o}{\hbar^2} \tag{7}$$

$$c^2 = \frac{2mU_o a^2}{\hbar^2}\,. \tag{8}$$

(c) Employ (5–8) for

$$c = 3\pi + 1 \tag{9}$$

to determine the energies E_j for which stationary states exist. How many states n are there? Solve the conditions (5–8) graphically.

(d) For (9) determine the normalized eigenstates $\psi(x, E_j)$, $j = 1, \ldots, n$ and plot the results.

This problem set needs to be handed in by Monday, March 31, 1997.