Physics 827 : Homework Set #5

Due Friday, Nov. 4, 2011, 1:00 pm in PRB M2043

Total point value of this set: 100 points

The 1-dimensional square well, $V(x) = \begin{cases} -V_0 & |x| \le a \\ 0 & |x| > a \end{cases}$ $(V_0 > 0)$

(1) $-V_0 \le E \le 0$ (bound states) (60 pts.)

(i) Show that the eigenvalue equation for the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x})$ has alternating even and odd solutions, with energy eigenvalues given by the solutions of

(15)
$$(ka)\tan(ka) = (\kappa a) \qquad \text{(even)}$$
$$(ka)\cot(ka) = -(\kappa a) \qquad \text{(odd)} \qquad (*)$$

where $\hbar\kappa = \sqrt{-2mE}$, $\hbar k = \sqrt{2m(E+V_0)}$. ($\kappa$ = kappa)

(ii) Defining the dimensionless parameter $\beta^2 = \frac{2(ma)(V_0 a)}{\hbar^2}$, show that $(\kappa a)^2 + (ka)^2 = \beta^2$ and that therefore

(5) the solutions for $\chi \equiv ka$ (χ = chi) and for $\left|\frac{E}{V_0}\right|$ depend only on β.

(iii) Solve the eigenvalue equations (*) graphically, by rewriting them as

$$f_{even}(\chi) \equiv \chi^2 \tan^2\chi = \beta^2 - \chi^2 \equiv F(\chi^2),$$
$$f_{odd}(\chi) \equiv \chi^2 \cot^2\chi = F(\chi^2), \qquad (**)$$

(20) plotting the functions f_{even}, f_{odd}, and F defined in (**) as functions of χ^2, and determining the intersection points between $f_{even/odd}$ and F for $\beta^2 = 30$. From the plot, read off the resulting values for $F \equiv (\kappa a)^2$. For $\beta^2 = 30$, how many bound states do you find?

(iv) Study analytically the limits $V_0 \to \infty$, a = const. (particle in a box) (5 pts.) and the case of a δ-fct. potential $V(x) = -g\,\delta(x)$,

(20) $g = \lim_{\substack{a\to 0 \\ V_0 \to \infty}} (2aV_0)$. In the latter limit, show that $\beta^2 \to 0$, $k \to \infty$,

$ka \to 0$, and $k^2 a \to mg/\hbar^2$, and that there are no odd solutions and exactly one even solution with energy eigenvalue $E = -\frac{mg^2}{2\hbar^2}$. So the attractive δ-fct. potential supports exactly one bound state.

(2) $E > 0$ (scattering states) (40 pts.)

(i) Writing $\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x < -a) \\ Ce^{ik'x} + De^{-ik'x} & (-a < x < a) \\ Fe^{ikx} + Ge^{-ikx} & (x > a) \end{cases}$

(20) show that

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \left(\cos(2k'a) - \frac{i\varepsilon'}{2}\sin(2k'a)\right)e^{2ika} & -\frac{i\eta'}{2}\sin(2k'a) \\ \frac{i\eta'}{2}\sin(2k'a) & \left(\cos(2k'a) + \frac{i\varepsilon'}{2}\sin(2k'a)\right)e^{-2ika} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

where $\varepsilon' = \frac{k'}{k} + \frac{k}{k'}$, $\eta' = \frac{k'}{k} - \frac{k}{k'}$, $\varepsilon'^2 + \eta'^2 = 4$.

(ii) Choosing the boundary condition $G = 0$ (no wave incident from the right), compute the transmission coefficient $T = \left|\frac{F}{A}\right|^2$ and the reflection coefficient $R = \left|\frac{B}{A}\right|^2$ as a function of β.

(10) You should find $T^{-1} = 1 + \frac{1}{4}\eta'^2 \sin^2(2k'a)$.

(iii) Plot T as a function of E/V_0 for a shallow potential with $\beta = 10$ and a deep potential with $\beta = 300$, showing in each case the first five "resonances" where $T = 1$.

(10) At which values for $(2k'a)$ does T exhibit maxima and minima? Can you interpret these physically? (Hint: think of wavelengths fitting into the potential well.) What are the limiting values of ε', η', and T as $E/V_0 \to \infty$?

4. *The Square Well.* Finally, we must discuss the so-called *square* (or rectangular) *well* (Figure 6.5). It is convenient to place the origin of the x axis in the center of the potential well so that $V(x)$ is again an even function of x:

$$V(x) = \begin{cases} -V_0 & \text{for } -a < x < a \quad (V_0 > 0) \\ 0 & \text{for } |x| \geq a \end{cases}$$

Depending on whether the energy is positive or negative, we distinguish two separate cases. If $E > 0$, the particle is unconfined and is scattered by the potential; if $E < 0$, it is confined and in a bound state. Assuming $-V_0 \leq E < 0$, we treat this last case first and set

$$\hbar k' = \sqrt{2m(E + V_0)}, \qquad \hbar\kappa = \sqrt{-2mE} \tag{6.44}$$

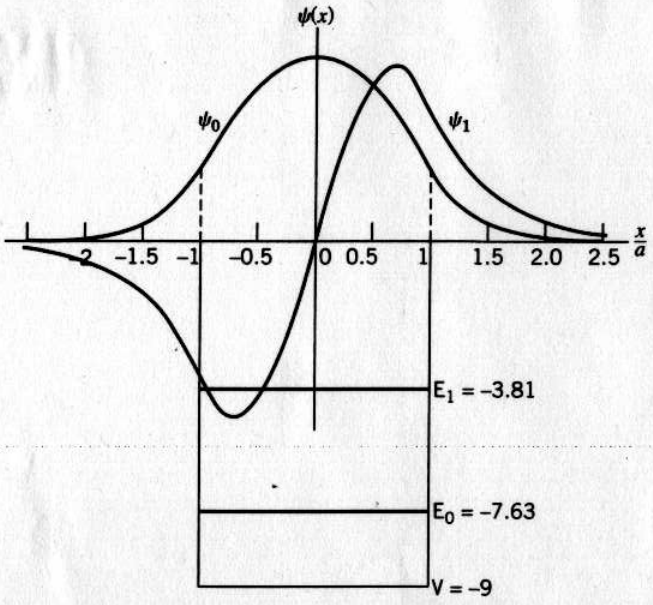

Figure 6.5. Square well potential of width $2a$ and depth V_0. For the choice of the parameter $\beta = 3$ there are two bound states. In units of $\hbar^2/2ma^2$, the well depth is $V_0 = 9$, and the energies for the two discrete states are $E_0 = -7.63$ and $E_1 = -3.81$. The ground and excited state eigenfunctions are equally normalized, but the scale is arbitrary.

The Schrödinger equation takes the form

$$\begin{aligned} &\frac{d^2\psi(x)}{dx^2} + k'^2\psi(x) = 0 \qquad \text{inside the well} \\ &\qquad\qquad\qquad\qquad\qquad\qquad (E < 0) \\ &\frac{d^2\psi(x)}{dx^2} - \kappa^2\psi(x) = 0 \qquad \text{outside the well} \end{aligned} \tag{6.45}$$

As for any even potential, we may restrict the search for eigenfunctions to those of definite parity.

Inside the well we have

$$\begin{aligned} \psi(x) &= A' \cos k'x \qquad \text{for even parity} \\ \psi(x) &= B' \sin k'x \qquad \text{for odd parity} \end{aligned} \tag{6.46}$$

Outside the well we have only the decreasing exponential

$$\psi(x) = C'e^{-\kappa|x|} \tag{6.47}$$

since the wave function must not become infinite at large distances.

It is necessary to join the wave function and its first derivative smoothly at $x = a$, that is, to require,

$$\begin{aligned} \lim_{\varepsilon\to 0} \psi(a - \varepsilon) &= \lim_{\varepsilon\to 0} \psi(a + \varepsilon) \\ \lim_{\varepsilon\to 0} \psi'(a - \varepsilon) &= \lim_{\varepsilon\to 0} \psi'(a + \varepsilon) \end{aligned}$$

Since an overall constant factor remains arbitrary until determined by normalization, these two conditions are equivalent to demanding that the *logarithmic derivative* of ψ,

$$\frac{1}{\psi(x)}\frac{d\psi(x)}{dx} = \frac{d \log \psi(x)}{dx} \tag{6.48}$$

be continuous at $x = a$. This is a very common way of phrasing the smooth joining conditions. Because of the reflection symmetry, the smooth joining conditions are automatically satisfied at $x = -a$ for both even and odd eigenfunctions.

The logarithmic derivative of the outside wave function, evaluated at $x = a$, is $-\kappa$; that of the inside wave functions is $-k' \tan k'a$ for the even case and $k' \cot k'a$ for the odd case.

The transcendental equations

$$\begin{aligned} k' \tan k'a &= \kappa \qquad \text{(even)} \\ k' \cot k'a &= -\kappa \qquad \text{(odd)} \end{aligned} \tag{6.49}$$

permit us to determine the allowed eigenvalues of the energy E.

The general symmetry considerations of Section 6.3 can also be extended to the solutions of the Schrödinger equation with negative values of k^2 and E. In (6.10) we need only replace k by $i\kappa$ and κ by ik'. The solution then takes the form

$$\psi(x) = \begin{cases} Ae^{-\kappa x} + Be^{\kappa x} & (x < -a) \\ Ce^{-ik'x} + De^{ik'x} & (-a < x < a) \\ Fe^{-\kappa x} + Ge^{\kappa x} & (a < x) \end{cases} \tag{6.50}$$

By requiring invariance under time reversal and imposing the principle of conservation of probability, we see that the matrix M, defined as in (6.24), must now be a *real* matrix with $\det M = 1$. The boundary conditions at large distances require that $A = G = 0$. In terms of the matrix M, we must thus demand that

$$M_{11} = 0 \tag{6.51}$$

and this equation yields the energy eigenvalues.

A simple graphical method aids in visualizing the roots of (6.49). We set

$$\chi = (k'a)^2, \quad \beta = \sqrt{\frac{2mV_0a^2}{\hbar^2}}, \quad (\kappa a)^2 + \chi = \beta^2$$

In Figure 6.6 we plot $F(\chi) = \beta^2 - \chi$ and

$$f_{\text{even}}(\chi) = \chi \tan^2 \sqrt{\chi} \text{ (if } \tan \sqrt{\chi} \geq 0) \qquad f_{\text{odd}}(\chi) = \chi \cot^2 \sqrt{\chi} \text{ (if } \tan \sqrt{\chi} \leq 0)$$

as functions of the positive independent variable χ. For the square well, the only pertinent parameter is the value of the dimensionless quantity β. The required roots are found by determining the intercepts of the straight line $F(\chi)$ with the curves f_{even} and f_{odd}. The ordinates $(\kappa a)^2$ of the intersection points are the scaled values of the bound-state energies.

By inspection of Figure 6.6, we can immediately draw several conclusions: All bound states of the well are nondegenerate; even and odd solutions alternate as the energy increases; the number of bound states is finite and equal to $N + 1$, if $N\pi < 2\beta \leq (N + 1)\pi$; if the bound states are labeled in order of increasing energy by a quantum number $n = 0, 1, \ldots N$, even values of n correspond to even parity, odd values of n correspond to odd parity, and n denotes the number of nodes; for any one-dimensional square well there is always at least one even state, but there can be no odd states unless $\beta > \pi/2$; and, the level spacing increases with increasing n.

As V_0 is allowed to increase beyond all bounds, two special cases merit discussion:

(a) Here we let $V_0 \to \infty$ while keeping the width of the square well finite, so that $\beta \to \infty$. For this infinitely deep potential well, the roots of the equations expressing the boundary conditions are now simply the asymptotes in Figure 6.6, or

$$\sqrt{\chi} = (n + 1)\,\pi/2 \qquad (n = 0, 1, 2, \ldots)$$

Hence,

$$\boxed{E + V_0 = (n + 1)^2 \frac{\pi^2\hbar^2}{8ma^2}} \tag{6.52}$$

The left-hand side of this expression, $E + V_0$, is the distance in energy from the bottom of the well and represents the kinetic energy of the particle in the well. Since

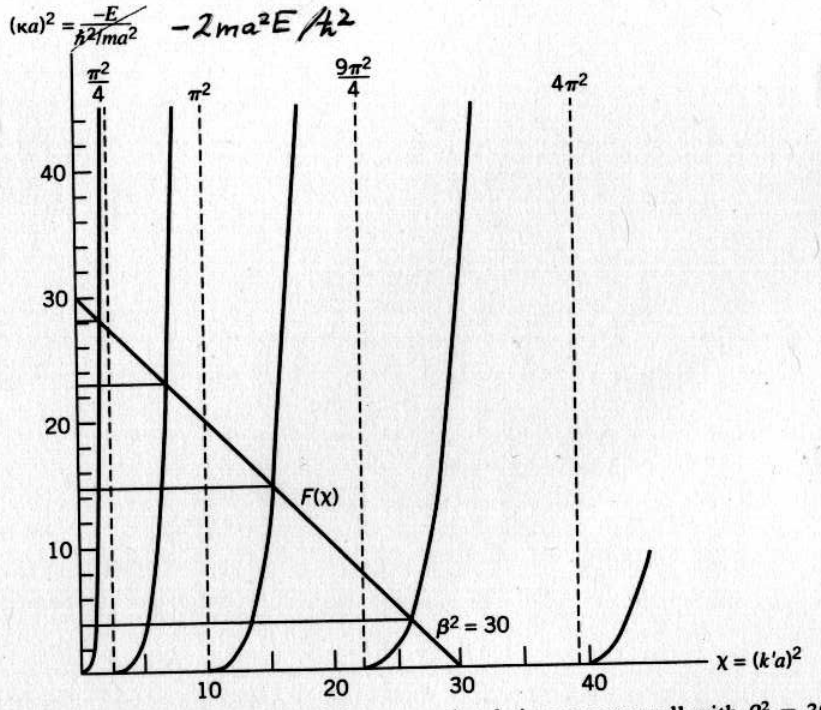

Figure 6.6. Graphic determination of the energy levels in a square well with $\beta^2 = 30$. The curves for $\tan \sqrt{\chi} \geq 0$ (f_{even}) alternate with those for $\tan \sqrt{\chi} \leq 0$ (f_{odd}). The ordinates of the intercepts are the binding energies in units of $\hbar^2/2ma^2$. The dashed-line asymptotes intersect the abscissa at the energy eigenvalues (6.52), again in units $\hbar^2/2ma^2$, for a particle confined to the box $-a \leq x \leq a$. This figure may be used as a template for estimating the bound-state energies for any one-dimensional square well: merely draw a parallel to the diagonal straight line $F(\chi) = \beta^2 - \chi$ for the desired value of β.

$E \to -\infty$ as $V_0 \to \infty$, it follows that $\kappa \to +\infty$; therefore, the wave function itself must vanish outside the well and at the endpoints $x = \pm a$. There is in this limit no condition involving the slope, which for an infinite potential jump can be discontinuous. Taking into account a shift V_0 of the zero of energy and making the identification $2a = L$, we see that the energy levels (6.52) for odd values of n coincide with the energy spectrum for a free particle whose wave function is subject to periodic boundary conditions (see Section 4.4). Note that the number of states is essentially the same in either case, since there is double degeneracy in (4.59) for all but the lowest level, whereas (6.52) has no degeneracy, but between any two levels (4.59) there lies one given by (6.52) corresponding to even values of n. There is, however, no eigenstate of the infinitely deep well at $E + V_0 = 0$ [corresponding to $n = 0$ in (4.59)], because the corresponding eigenfunction vanishes.

(b) Another interesting special case arises if V_0 tends to infinity as a tends to zero, but in such a way that the product V_0a remains finite. As in (6.17), we denote the area under the potential by $g = \lim(2V_0a)$, but instead of being a repulsive barrier the potential is now the attractive delta function well,

$$V(x) = -g\delta(x) \tag{6.53}$$

In this limit $k' \to \infty$, but $k'a \to 0$, and $k'^2 a \to 2mV_0 a/\hbar^2$ and remains finite. There are no odd solutions of (6.49) in this case, but there is one even root given by

$$k'^2 a = \kappa$$

or

$$\boxed{E = -\frac{mg^2}{2\hbar^2}} \tag{6.54}$$

Thus, the attractive one-dimensional delta function well supports only one bound state.

This conclusion can be verified directly from the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - g\delta(x)\psi(x) = E\psi(x) \tag{6.55}$$

if we integrate this equation from $x = -\varepsilon$ to $x = +\varepsilon$ and then take the limit $\varepsilon \to 0$. The result is

$$\lim_{\varepsilon\to 0} \psi'(x)\Big|_{-\varepsilon}^{+\varepsilon} + \frac{2mg}{\hbar^2}\psi(0) = 0 \tag{6.56}$$

From (6.47) we see that $\psi(0) = C'$ and

$$\lim_{\varepsilon\to 0} \psi'(x)\Big|_{-\varepsilon}^{+\varepsilon} = -2C'\kappa$$

Inserting these values in (6.56), we obtain

$$\kappa = \frac{mg}{\hbar^2} \tag{6.57}$$

which is equivalent to the energy equation (6.54).

To conclude this chapter we discuss briefly what happens to a particle incident from a great distance when it is scattered by a square well. Here $\boxed{E > 0}$. Actually, this problem has already been solved. We may carry over the results for the potential barrier, replacing V_0 by $-V_0$ and κ by ik', where $\hbar k' = \sqrt{2m(E + V_0)}$. Equation (6.12) becomes

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \left(\cos 2k'a - \frac{i\varepsilon'}{2}\sin 2k'a\right)e^{2ika} & -\frac{i\eta'}{2}\sin 2k'a \\ \frac{i\eta'}{2}\sin 2k'a & \left(\cos 2k'a + \frac{i\varepsilon'}{2}\sin 2k'a\right)e^{-2ika} \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix} \tag{6.59}$$

where

$$\varepsilon' = \frac{k'}{k} + \frac{k}{k'}, \qquad \eta' = \frac{k'}{k} - \frac{k}{k'}, \quad \varepsilon'^2 - \eta'^2 = 4. \tag{6.60}$$

Equation (6.59) defines the matrix M for the square well if the energy is positive.

The transmission coefficient T is obtained from (6.59) by choosing stationary states with $G = 0$ (no wave incident from the right), and writing

$$\frac{F}{A} = \frac{1}{M_{11}} = S_{12} = \sqrt{T}e^{-i\phi} \tag{6.61}$$

This expression defines a phase shift ϕ between the transmitted and the incident wave. From the properties of the S matrix in Section 6.3, or directly from (6.59), we find for the relation between the reflected and the incident wave:

$$\frac{B}{A} = \frac{M_{21}}{M_{11}} = S_{11} = \sqrt{1 - T}e^{-i(\phi \pm \pi/2)} \tag{6.62}$$

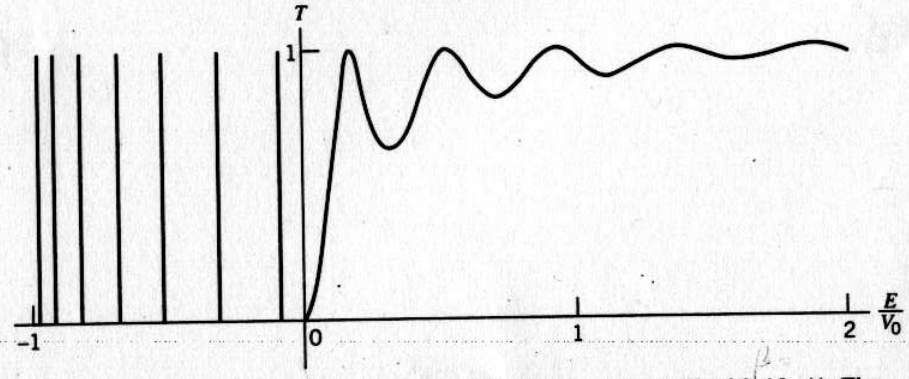

Figure 6.7. Transmission coefficient T versus E/V_0 for a square well with $13\pi/4$. The spikes on the left are at the positions of the seven discrete bound-state energy levels.

For the square well,

$$T = \frac{1}{|M_{11}|^2} = \frac{1}{\cos^2 2k'a + \frac{\varepsilon'^2}{4}\sin^2 2k'a} \tag{6.63}$$

As $E \to \infty$, $\varepsilon' \to 2$, and $T \to 1$, as expected. As a function of energy, the transmission coefficient rises from zero, fluctuates between maxima ($T = 1$) at $2k'a = n\pi$ and minima near $2k'a = (2n + 1)\frac{\pi}{2}$, and approaches the classical value $T = 1$ at the higher energies. Figures 6.7 and 6.8 show this behavior for two different values of

β. The maxima occur when the distance $4a$ that a particle covers in traversing the well and back equals an integral number of de Broglie wavelengths, so that the incident wave and the waves that are reflected inside the well are in phase reinforcing each other. If the well is deep and the energy E low (β and $\varepsilon' \gg 1$), the peaks stand out sharply between comparatively flat minima (see Figure 6.8). When the peaks in the transmission curve are pronounced they are said to represent *resonances*.

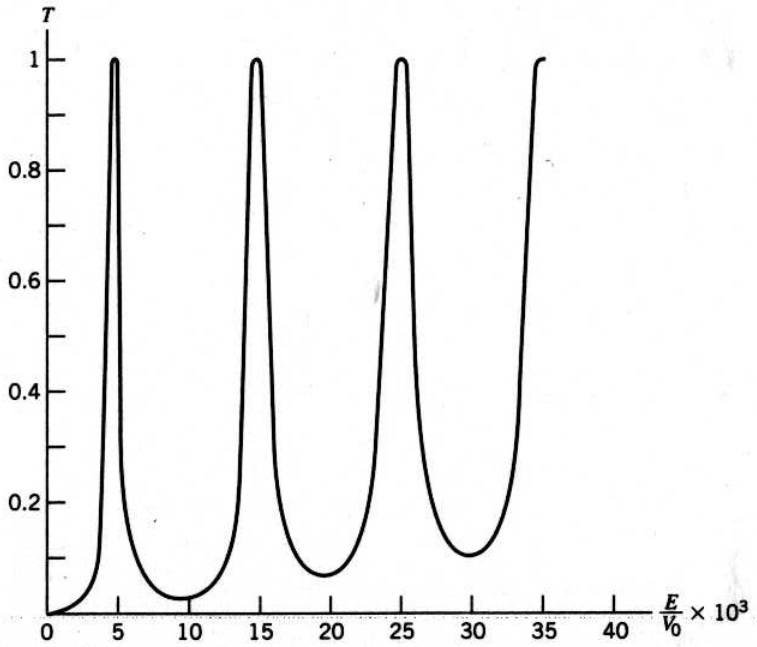

Figure 6.8. Transmission coefficient T versus E/V_0 for a deep square well with $\beta = 315$. As E increases, the resonances become broader.