PH 401 Problem Set # 5

Due: Wednesday, October 29, 2003

In this problem set you will carry out the alternative analysis of the square well described in footnote 27 on page 63 of Griffiths. Since parity commutes with the Hamiltonian (because the potential is symmetric), we should be able to simultaneously diagonalize the Hamiltonian and parity, that is, find eigenstates of the Hamiltonian that are also either even or odd functions. While we did this for the bound states, we did not for the scattering states. One way to think about it is that in the presentation in the book, there are two scattering solutions for a given energy: one is the wave that comes in from the left and the other is the one that comes in from the right. The parity eigenstates are linear combinations of these two cases: the even state comes in with equal components from left and right, and the odd state comes in with equal and opposite components from left and right.

In this process, you will learn about a very useful tool in quantum mechanics and discover experimentally a fundamental theorem governing its behavior.

1. Start by doing Griffiths 2.28. Set up Mathematica (or your favorite graphing program) so that if the width a and depth V_0 are both specified numerically, you can graphically estimate both the odd and even bound states (you'll need this later). To make life simpler, work in units of $\frac{\sqrt{2m}}{\hbar}$. In other words, set this quantity to one everywhere in all of your numerical calculations, both in this and subsequent problems. (Of course, in the analytic formulae you are asked to calculate, you should keep it around.)

2. Now let's find the scattering states that are also parity eigenstates. Let's start with the odd states. Outside the potential (that is, for $|x| > a$), we just have the free Hamiltonian. As you found on a previous problem set, you can choose eigenstates of the Hamiltonian with negative parity in the form of $\psi(x) = \sin kx$ with $k > 0$. Because we are only looking at $|x| > a$, however, we have to be a little more general. Consider a solution of the form

$$\psi_{\text{out}}(x) = \sin\left(kx + \text{sgn}(x)\delta_A(k)\right)$$

where $\delta_A(k)$ is a real number independent of x but possibly dependent on k, called the *phase shift*. (The "A" indicates that we are dealing with the antisymmetric case.) Here $\text{sgn}(x) = x/|x|$ is just the sign of x, necessary to ensure that the function is odd. Of course, this is not a solution to the free Hamiltonian everywhere (unless $\delta_A(k) = 0$), because at the origin it has a kink due to the $\text{sgn}(x)$, but in this case we never encounter that region.

(a) Show that $\sin(kx + \operatorname{sgn}(x)\delta_A(k))$ solves the eigenvalue equation outside the potential and find the relationship between k and E (which should look familiar).

(b) Inside the potential (that is, for $|x| < a$), we have a solution of the form

$$\psi_{\text{in}}(x) = C_A(k) \sin qx$$

There can't be a $\cos qx$ because it wouldn't be odd, and there can't be a phase shift because there would be a kink at the origin. $C_A(k)$ is just a normalization constant (which can depend on k). Find q in terms of k and V_0, and then match up $\psi(x)$ and $\psi'(x)$ at the boundary $x = a$ to solve for the two unknowns $C_A(k)$ and $\delta_A(k)$ in terms of k, V_0 and a. (By the symmetry of the problem, once you match up the boundary conditions at $x = a$, they will automatically be satisfied at $x = -a$.)

(c) Repeat this analysis for the symmetric wavefunctions, which outside are of the form

$$\psi_{\text{out}}(x) = \cos(k|x| + \delta_S(k))$$

and inside are of the form

$$\psi_{\text{in}}(x) = C_S(k) \cos qx$$

(d) For some selected values of V_0 and a, plot both phase shifts as functions of k and use the graphical method to find the number of symmetric and antisymmetric bound states. Be sure to consult the hints below before carrying out your numerical calculation. Choose one of your examples with $V_0 < 0$; in that case we have a repulsive potential, which has no bound states (but your formulae for the phase shifts are unchanged — just plug in the negative value of V_0). Do at least two cases with $V_0 > 0$.

(e) There is a relationship, called *Levinson's theorem*, between each phase shift at $k = 0$ and the corresponding number of bound states. Find this relationship experimentally from your numerical examples. Note that Levinson's theorem is slightly different between the symmetric and antisymmetric cases.

Hint: Again, set $\dfrac{\sqrt{2m}}{\hbar} = 1$ in the numerical calculation.

Hint: Since the phase shift is a phase, we can always add multiples of 2π to it without changing anything. In fact, if we add an odd multiple of π all we do is change the sign of the wavefunction, so it's really only defined up to adding any multiple of π. You should see this in your calculation because the phase shifts you found should be the arctangents or arccotangents of something, and we have to arbitrarily pick which of the infinite set of angles differing by π to use.

However, for Levinson's theorem to work, we will need to specify the phase shift uniquely. Here is how to do it:

- Demand that the phase shift go to zero as $k \to \infty$.
- Demand that the phase shift be a continuous function of k.

Probably the phase shift you get out of Mathematica (or your favorite graphing program) will not look like this — instead it will jump. Deal with this either by sketching on the graph what the phase shift would look like if the different segments were shifted by π to make it continuous, or else by tricking Mathematica into giving you the form you want by using the fundamental theorem of calculus:

$$\delta(k) = \int_{\infty}^{k} \delta'(k')dk' \tag{1}$$

where $\delta'(k)$ is the derivative of the phase shift with respect to k. In other words, you compute $\delta'(k')$ by hand from your formula for $\delta(k)$, and then get Mathematica to give you back $\delta(k)$ using the above formula. By construction, it will vanish at infinity and be continuous.

Here is a Mathematica snippet that might be helpful for implementing this trick:

```
a = (your choice)
v0 = (your choice)
deltaA[k_] := (your result for the antisymmetric phase shift)
deltaS[k_] := (your result for the symmetric phase shift)
fixup[f_] := Function[k, NIntegrate[f'[p], {p, 50/a, k}]]
Plot[fixup[deltaA][k],{k,0,8/a}]
Plot[fixup[deltaS][k],{k,0,8/a}]
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where $50/a$ is the "infinite" upper limit, which just needs to be much larger than 1. (Mathematica allows you to specify the upper limit as Infinity, but this is not always reliable numerically.) Note that the range of interesting values of k goes like the inverse distance $1/a$. Putting the $\hbar$ back in, this means that the interesting momenta $p = \hbar k$ are those such that $p \cdot a \approx \hbar$.

Hint: Since the phase shift is a phase, it may help to divide it by π in order to see what it is doing.

3. We can define the phase shift for any symmetric potential $V(x)$ that vanishes fast enough at large $|x|$, since if the potential is very small when we are far

away, the solutions far away will be arbitrarily close to the form of our $\psi_{\text{out}}(x)$ functions above. However, it might not be practical to actually calculate the phase shifts exactly in the general case. The *Born approximation* to the phase shift is given by

$$\delta_A^{\text{Born}}(k) = -\frac{2m}{\hbar^2} \cdot \frac{1}{2k} \int_{-\infty}^{\infty} V(x) \sin^2 kx \, dx$$

in the antisymmetric channel and

$$\delta_S^{\text{Born}}(k) = -\frac{2m}{\hbar^2} \cdot \frac{1}{2k} \int_{-\infty}^{\infty} V(x) \cos^2 kx \, dx$$

in the symmetric channel. Evaluate the Born approximation for the square well case. For one of your numerical examples, plot the Born approximation together with the full phase shift in both channels. Where, as a function of k, does the Born approximation work well?

Hint: Remember that the potential for the square well is $V(x) = -V_0$ for $|x| < a$ and zero elsewhere — don't forget the minus sign.

Hint: Once again, you should set $\frac{\sqrt{2m}}{\hbar} = 1$ in the numerical calculation (which is why I've separated the square of this term out explicitly in the formulae above).

4. Finally, let's connect this calculation to the standard approach done in class and in Griffiths. The ratio of the amplitude of the transmitted wave to the amplitude of the incident wave is given by Eq. (2.150) as

$$t(k) = \frac{e^{-2ika}}{\cos 2qa - i\frac{\sin 2qa}{2qk}(k^2 + q^2)}$$

and the ratio of the amplitude of the reflected wave to the amplitude of the incident wave is given by Eq. (2.149) as

$$r(k) = i\frac{\sin 2qa}{2qk}(q^2 - k^2)t(k)$$

Show that

$$r(k) = \frac{1}{2}\left(e^{2i\delta_S(k)} - e^{2i\delta_A(k)}\right)$$

and

$$t(k) = \frac{1}{2}\left(e^{2i\delta_S(k)} + e^{2i\delta_A(k)}\right)$$

Hint:

$$\arctan x = \frac{1}{2i}\ln\frac{1+ix}{1-ix} \qquad \operatorname{arccot} x = \arctan\frac{1}{x}$$

Here is how to interpret this result (you don't have to do anything with this information except admire the beautiful interconnectedness of things). In the original calculation, we can think of our basis as consisting of two states for a given energy: the waves moving to the left and the waves moving to the right. The scattering can be summarized by the S-matrix

$$S = \begin{pmatrix} t(k) & r(k) \\ r(k) & t(k) \end{pmatrix}$$

as follows: If we multiply this matrix by the vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, representing an incoming wave moving to the right, what comes out is the linear combination $\begin{pmatrix} t(k) \\ r(k) \end{pmatrix}$. That is, $t(k)$ tells us the component still moving to the right (the transmitted wave), and $r(k)$ tells us how much of a component moving to the left we pick up (the reflected wave). Similarly, a left-moving incident wave $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ turns into $\begin{pmatrix} r(k) \\ t(k) \end{pmatrix}$. Again, $t(k)$ tells us how much continues to the left and $r(k)$ tells us how much is reflected back to the right (since the potential is symmetric, the transmission and reflection is the same regardless of which way we come in from). Because $|r(k)|^2 + |t(k)|^2 = 1$, this matrix is unitary, and thus the probability to go somewhere remains one.

The calculation you have just done corresponds to using a different orthonormal basis for this two-dimensional subspace. The symmetric channel is $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, an equal combination of left- and right-moving waves. The antisymmetric channel is $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, an equal and opposite combination of left- and right-moving waves. These states are still eigenstates of the Hamiltonian (since they are just linear combinations of eigenstates with the same energy E), but they are also eigenstates of parity. Since parity commutes with the Hamiltonian, it's conserved and these states can't mix together under time evolution. Thus in this basis the S-matrix is diagonal. In particular, the calculation you have just done shows that in this basis S becomes

$$S = \begin{pmatrix} e^{2i\delta_S(k)} & 0 \\ 0 & e^{2i\delta_A(k)} \end{pmatrix}$$

That is, each channel just picks up a phase given by twice the phase shift you found.

The S-matrix is described in more detail in section 2.7 of Griffiths, though he uses arcane conventions in which $r(k)$ goes on the diagonal and $t(k)$ on the off-diagonal (I've done it the other way around).