Details from Lecture
Sept. 18, 2003

1 Phase shifts

In lecture today, we talked about phase shifts. I wanted to provide you all with a few more details since you'll need them for your homework. First of all, we define phase shifts from the asymptotic form of the wave function:

$$\psi \longrightarrow A' e^{i(kx+\phi)}. \tag{1}$$

Notice that there's a difference of a minus sign relative to what I wrote on the board. *Use the above definition.*

For the finite attractive square well example we did in class, the transmitted wave function is

$$\psi(x) = \frac{e^{-2ika}}{\cos 2k'a - \frac{i\varepsilon'}{2}\sin 2k'a} A e^{ikx}. \tag{2}$$

The variables here are defined as

$$k = \sqrt{\frac{2m}{\hbar^2}E}$$
$$k' = \sqrt{\frac{2m}{\hbar^2}(E+V_0)}$$
$$\varepsilon' = \frac{k'}{k} + \frac{k}{k'}.$$

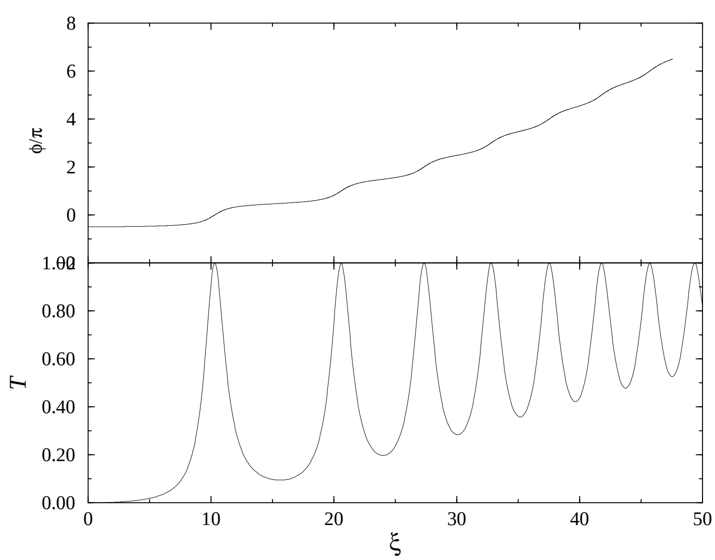
Comparing the wave functions in Eqs. (1) and (2), we see that the phase shift is

$$\phi = 2ka - \tan^{-1}\left(\frac{\varepsilon}{2}\tan 2k'a\right). \tag{3}$$

Defining the dimensionless energy parameter $\xi = ka$ and the dimensionless potential parameter $\beta = \sqrt{2mV_0/\hbar^2}a$ gives

$$\phi = 2\xi - \tan^{-1}\left[\frac{1}{2}\left(\frac{\sqrt{\xi^2+\beta^2}}{\xi} + \frac{\xi}{\sqrt{\xi^2+\beta^2}}\right)\tan(2\sqrt{\xi^2+\beta^2})\right]. \tag{4}$$

Note that ξ is defined differently than in class. The present definition relates ξ to E more simply. The phase shift is plotted in the graph below for $\beta = 100$. Two things should be pointed out about this figure. First, the phase shift has been corrected



for the π ambiguity inherent in $\tan -1$; and second, the "background" phase shift $2ka = 2\xi$ has not been included. This background phase shift is just the phase that a freely propagating plane wave e^{ikx} would have accumulated over the distance $2a$ across the well without a potential.

Also shown in this figure is the transmission coefficient T. It's clear that there are several resonances in this energy range and that for each resonance, the phase shift rises by π. Both the phase shift and the transmission coefficient are calculated from the same expression in Eq. (2), so maybe it's no surprise that they are so closely related.

2 Double well systems

In lecture, we also talked about double well systems and how their energies are related to the energies of the two wells individually. I got hung up on the derivation of the energy splitting, and I wanted to clear up the problem.

In class, we got to the following expression for the ground (+) and first excited (−) energies:

$$E_{\pm} = \varepsilon_0 + \frac{\langle\phi_1|V_2|\phi_1\rangle \pm \langle\phi_2|V_2|\phi_1\rangle}{1 \pm \langle\phi_1|\phi_2\rangle}. \tag{5}$$

$|\phi_i\rangle$ are the ground states of their respective wells separately, and ε_0 is the corresponding energy (identical for both because the wells are assumed identical). This expression is correct, my discussion of the two matrix elements in the numerator was *not* correct.

The matrix element $\langle\phi_2|V_2|\phi_1\rangle$ will always be bigger than $\langle\phi_1|V_2|\phi_1\rangle$ because phi_2 is always larger in the second well than is ϕ_1. Moreover, since the well is attractive, both matrix elements will be negative (the overlap of ϕ_1 and ϕ_2 in the denominator is always positive). So, to a good approximation, the energies are

$$E_{\pm} \approx \varepsilon_0 \mp \frac{|\langle\phi_2|V_2|\phi_1\rangle|}{1 \pm \langle\phi_1|\phi_2\rangle}. \tag{6}$$

So, the even parity state (+) always has a lower energy than the odd parity (−) state when constructed as linear combinations of individual well solutions. That's good, since we expect the ground state of any system to be nodeless!