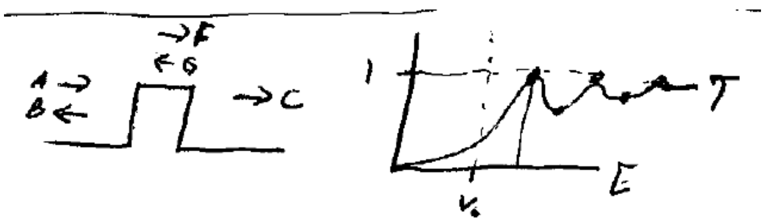
Lecture 14: Resonant Scattering and the S-Matrix

1 Last Time

We looked at:

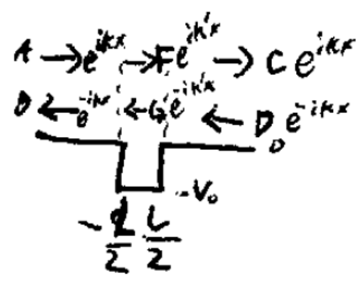


Note: Resonances at $k_2 L = n\pi, T \to 1$. [at $k_2 L = (n + \frac{1}{2})\pi$: $R \to \frac{V_0^2}{(2E - V_0)^2}$]

- N wavelengths precisely fit inside
- Subsequent reflections exactly in/out of phase
- Perfect transmission!!!

Note: When $k_2 L = (n + \frac{1}{2})\pi, T \to \frac{4E(E-V_0)}{(2E-V_0)^2}, R \to \frac{V_0^2}{(2E-V_0)^2}$.

2 A More Interesting Example



Definitions:

$$k = \sqrt{\frac{2m}{\hbar^2} E} \tag{1}$$

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

The wavefunction, ϕ_E, is:

$$Ae^{ikx} + B^{-ikx} \tag{3}$$

for $x < -\frac{L}{2}$,

$$Fe^{ik'x} + G^{-ik'x} \tag{4}$$

for $-\frac{L}{2} < x < \frac{L}{2}$, and

$$Ce^{ikx} + D^{-ikx} \tag{5}$$

for $\frac{L}{2} < x$.

Again, matching conditions at $x = \pm\frac{L}{2}$, determine $\begin{pmatrix} F \\ G \end{pmatrix}$ in terms of $\begin{pmatrix} A \\ B \end{pmatrix}$ and $\begin{pmatrix} F \\ G \end{pmatrix}$ in terms of $\begin{pmatrix} C \\ D \end{pmatrix}$.

$\begin{pmatrix} A \\ B \end{pmatrix} = (\mathrm{M})\begin{pmatrix} C \\ D \end{pmatrix}$ or $\begin{pmatrix} C \\ D \end{pmatrix} = (M^{-1})\begin{pmatrix} A \\ B \end{pmatrix}$

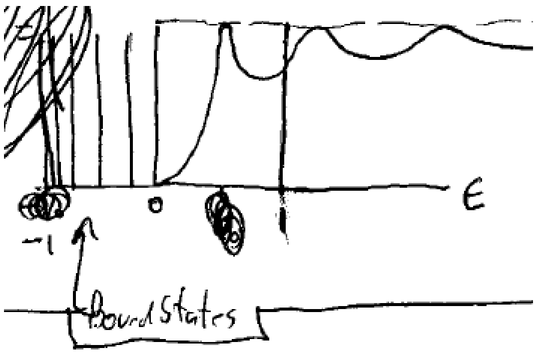
Rather than solve it all over again, recognize that it is the same as the case we had before, with $V_0 \rightarrow -V_0$ and $k' = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$. This gives us:

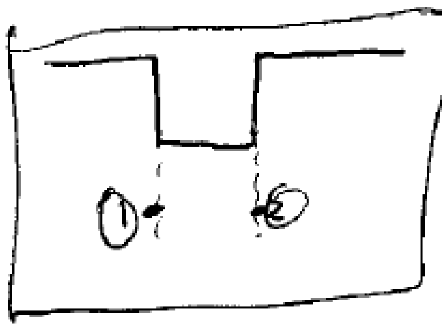
$$T = \frac{1}{1 + \frac{1}{4\epsilon(\epsilon+1)} \sin^2 \sqrt{g_0^2(\epsilon + 1)}} \tag{6}$$

where, again, $\epsilon = \frac{E}{V_0}$ and $g_0^2 = \frac{2m}{\hbar^2} V_0 L^2$

This is called the Ramsauer Effect.

Again, we have resonances! At $k'L = N\pi, \sin^{k'L} = 0 \Rightarrow T = 1$. Why?





- Think about it this way: how do you transmit across the well? From (1) to (2) in the figure below?

  Well, you can treat this as two independent step scatterings. First, how do you get to (2)? Well, you can transmit twice (once into the well, evolve $e^{ik'L}$, then out of the well) or ($t_{\rightarrow}$, evolve, $r_{\leftarrow}$, evolve, $r_{\rightarrow}$, evolve, $t_{\rightarrow}$) or (trrrrt) or...

  t across the well can therefore be written as:

$$t^* e^{ik'L} t + t^* e^{ik'L} r e^{ik'L} r^* e^{ik'L} t + ... \tag{7}$$

$$= |t|^2 e^{ik'L} (1 + |r|^2 e^{2ikL} + |r|^4 e^{4ikL} + ...) \tag{8}$$

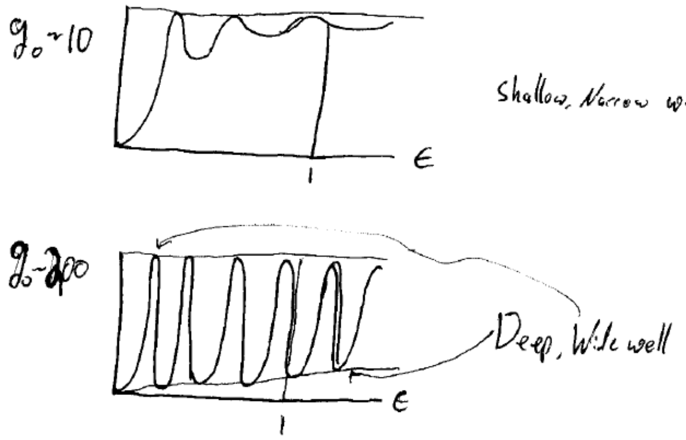
$$= |t|^2 e^{ik'L} \frac{1}{1 - |r|^2 e^{2ik'L}} \tag{9}$$

$$= \frac{|t|^2}{e^{-ik'L} - |r|^2 e^{ik'L}} = \frac{-T}{(1-T)e^{ik'L} - e^{-ik'L}} = \frac{-T}{2i \sin k'L - T e^{ik'L}} \tag{10}$$

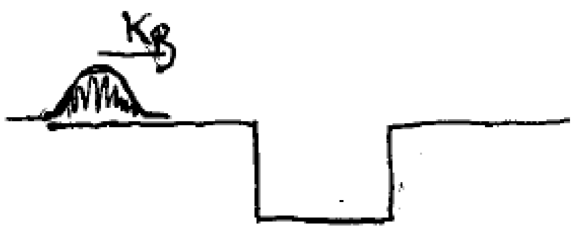
  Therefore,

$$t_{tot} = \frac{1}{e^{ik'L} - \frac{2i}{T}\sin k'L} \Rightarrow T_{tot} = \frac{1}{1 + \frac{(k^2-k'^2)^2}{4k^2k'^2}\sin^2 k'L} \tag{11}$$

So, resonant peaks reflect constructive interference from multiple internal scatterings inside the potential.



- It's illuminating to consider the motion of a simple wavepacket thrown from left at the square well:



$$\psi_{incident} = \int_0^\infty \frac{dk}{\sqrt{2\pi}} f(k) e^{i(kx-\omega_k t)} \tag{12}$$

where $\omega_k = \frac{\hbar k^2}{2m}$. $f(k)$ is peaked at k_0, corresponding to v_0, E_0. The wavepacket moves with the group velocity ω. So, $x = \frac{\hbar k_0}{m} t = v_0 t$.

- In the presence of the well, $\psi_{incident}$ is not the full wavefunction.

For $x < -\frac{L}{2}$, there is also a reflected wave, and for $x > \frac{L}{2}$ there is a transmitted wave. As we've seen, for a given k,

$$\frac{C}{A} = \sqrt{T}e^{-k\phi} \tag{13}$$

$$\frac{B}{A} = \sqrt{1-T}e^{-i\phi \pm i\frac{\pi}{2}} \tag{14}$$

for some phase ϕ - called the phase shift. We can then use superposition to write the reflected wavepacket as

$$\psi_{ref} = \int_0^\infty \frac{dk}{\sqrt{1-T}} f(k) e^{-i(kx - i\omega t + \phi + \frac{\pi}{2})} \tag{15}$$

The peak of this wavepacket is determined by

$$\frac{d}{dk_0}[k_0 x + \omega(k_0)t + \phi(k_0)] = 0 \Rightarrow x = -v_0(t + \hbar\frac{\partial\phi}{\partial E}(k_0)) \tag{16}$$

What this is telling us is that the time delay between the arrival of the incident peak and the reflected peak at the left edge of the well is $\frac{L}{V_0} = -\hbar\frac{\partial\phi}{\partial E}(k_0)$.

- Finally, on the right of the well, there is also a transmitted wave,

$$\psi_{transmitted} = \int_0^\infty \frac{dk}{\sqrt{T}} f(k) e^{i(kx - \omega t \phi)} \tag{17}$$

whose peak, at $\partial_{k_0}[k_0 x - \omega_{k_0} t - \phi(k_0)] - 0$, moves as

$$x_t = v_0[t + \hbar\frac{\partial\phi}{\partial E}(k_0)] \tag{18}$$

Interpretation: In absence of well, peak moves at constant speed v_0. In well, it goes faster, and gets out sooner. For a deep well, and low v_0 [the conditions for resonances] this time interval should be L/v_0. Thus we have a classical guess, $\hbar\frac{\partial\phi}{\partial E}(k_0)$ goes as $\frac{L}{v_0}$. Is this right?

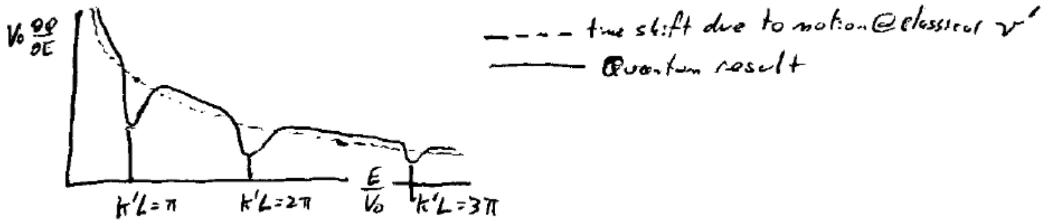
Let's be explicit for our square well. From above, we have

$$\phi = k'L - \arctan\frac{k'^2 + k^2}{2kk'}\tan k'L \tag{19}$$

Near resonance, $k'L \sim N\pi$, this gives

$$\hbar \frac{\partial \phi}{\partial E} = \frac{L}{2 v_0} \left(\frac{1}{1 + \frac{E}{V_0}} \right) \tag{20}$$

which is off by a factor of two! In general,



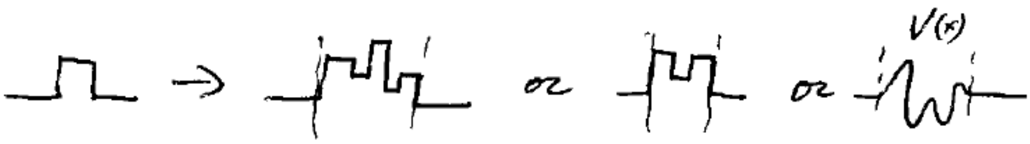
Note: big slow-down at resonance! Why? Well, why resonance? Because MANY BOUNCES!! Can estimate time spent bouncing in well, reproduces this "$\frac{1}{2}$" precisely.

Note: for the well, the phase shift was positive: speed up! For the barrier, the phase shift will be negative: slow down! Even the **sign** of the phase shift is revealing: sign of potential! There's lots of physics in T, R, δ!

3 Generalizing Scattering Problems

So far we've been setting up scattering problems, setting a prefaactor equal to zero, and using matching. It's illuminating to generalize in two ways:

1. Clearly, the same kind of move works if



   we just have lots more matching conditions. Thus, as for Step or Barrier, we can always solve the S.E. in V(x) to deduce matching conditions between $\begin{pmatrix} A \\ B \end{pmatrix}$ and $\begin{pmatrix} C \\ D \end{pmatrix}$!

2. We've set D=0 to model sending things in only from the left. $A \Rightarrow \begin{pmatrix} B \\ C \end{pmatrix}$. But, more physically, any values of any two of A, B, C, D specify a valid solution -

indeed $\hat{E}\phi_E = E\phi_E$ is a 2nd order ODE, so has 2 integration constants. Physically, why specify A and D? Why not A and C, or B and D? **Because A, D are in-going, while B, C are outgoing.**

Thus, the most natural thing to do is specify $\begin{pmatrix} A \\ D \end{pmatrix}$ and compute $\begin{pmatrix} B \\ C \end{pmatrix}$. By linearity, and also from experience, we can always write:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} \delta_{11}\delta_{12} \\ \delta_{21}\delta_{22} \end{pmatrix}\begin{pmatrix} A \\ D \end{pmatrix} \tag{21}$$

This generalizes naturally to 3D! (and 100D!)

The square matrix is called the "S-Matrix" ($\hat{S}$)for "scattering". Now we study its properties.

4 Properties of the S-Matrix, $\hat{S}$

1. Stuff doesn't disappear! What goes in, must come out.

$$|A|^2 + |D|^2 = |B|^2 + |C|^2 \tag{22}$$

is equivalent to the statement that $J_x =$ constant. In matrix notation,

$$(B^*C^*)\begin{pmatrix} B \\ C \end{pmatrix} = (A^*D^*)\begin{pmatrix} A \\ D \end{pmatrix} \tag{23}$$

But $\begin{pmatrix} B \\ C \end{pmatrix} = S\begin{pmatrix} A \\ D \end{pmatrix}, (BC) = (AD)S^T, (B^*C^*) = (A^*D^*)S^{T*}$.

$(A^*D^*)S^{T*}S\begin{pmatrix} A \\ D \end{pmatrix} = (A^*D^*)\begin{pmatrix} A \\ D \end{pmatrix} \Rightarrow S^{T*} \cdot S = 1.$

$$S^{\dagger}S = 1 \equiv Sisaunitarymatrix \tag{24}$$

- Physically, this preserves probability
- Mathematically, eigenvalues are phases: $s_1 = e^{i\phi_1}, s_2 = e^{i\phi_2}$

This leads to the following constraints on the S-Matrix elements:

$$|s_{11}| = |s_{22}|, |s_{12}| = |s_{21}|, |s_{11}|^2 + |s_{12}|^2 = 1, s_{11}s_{12}^* + s_{21}s_{22}^* = 0 \tag{25}$$

2. Since V(x) is real, the SE has time-reversal symmetry, and so

$$\psi = \begin{cases} A^* e^{-ikx} + B^* e^{ikx} & \text{Left;} \\ ... & \text{Inside;} \\ C^* e^{-ikx} + D^* e^{ikx} & \text{Right} \end{cases}$$

is also a solution. But this is equivalent to exchanging A with B^*, and C with D^*, so it must also be true that

$$\begin{pmatrix} A^* \\ D^* \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} B^* \\ C^* \end{pmatrix} \tag{26}$$

Together with the above, this gives

$$S^* S = 1 \tag{27}$$

or equivalently,

$$S^T = S \tag{28}$$

So, if we have time-reversal invariance, $\hat{S}$ is a symmetric unitary matrix, and $s_{12} = s_{21}$.

3. If we have parity, $x \to -x$ (eg, if V(x) is even) then, as above, we haveanother solution with $A \leftrightarrow C, B \leftrightarrow D$.

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} D \\ A \end{pmatrix} \leftrightarrow \begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} s_{22} & s_{21} \\ s_{12} & s_{11} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} \tag{29}$$

Parity implies $s_{11} = s_{22}$ and $s_{12} = s_{21}$.

4. Thus, if we have T, P, and unitarity,

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \tag{30}$$

with $|s_{11}|^2 + |s_{12}|^2 = 1$, and $s_{11} s_{12}^* + s_{11}^* s_{12} = 0$

Now, it's helpful to recall what the s_{ij} means.

$$S = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \tag{31}$$

1. Unitarity: $R+T=1$, $|\tilde{t}|=|t|$, $|\tilde{r}|=|t|, r\tilde{t}^*+t\tilde{r}^*=0$
2. Time-reversal: $t=\tilde{t}$
3. Parity: $r=\tilde{r}$

$$S = \begin{pmatrix} \sqrt{1-T}e^{i(\delta\pm\frac{\pi}{2})} & \sqrt{T}e^{i\delta} \\ \sqrt{T}e^{i\delta} & \sqrt{1-T}e^{i(\delta\pm\frac{\pi}{2})} \end{pmatrix} \tag{32}$$

Note: True for every example we studied. But more general - follows from U, T, and P!

Key: the $\hat{S}$-Matrix contains all physical information about any localized potential V(x). For example, when D=0, we can recover the r and t amplitudes, including ϕ.

Remarkably, even knows about bound states!

In this case, $E<0$, so $k\to i\alpha$. For normalizability, $A=D=0$. You might think this kills B, C, since $\begin{pmatrix} B \\ C \end{pmatrix} = S\begin{pmatrix} A \\ D \end{pmatrix}$, but not if S blows up!

For example, with this kind of well,

$$S_{21}=t=\frac{2kk'e^{-ikL}}{2kk'\cos k'L-i(k^2+k'^2)\sin k'L} \tag{33}$$

When $E\to -E, k\to i\alpha$, the denominator $\to i2k'\alpha\cos k'L - i(k'^2-\alpha^2)\sin k'L$. The denominator becomes 0 when $\cot k'L=\frac{k'^2-\alpha^2}{2\alpha k'}\leftrightarrow \frac{k'L}{2}\tan\frac{k'L}{2}=\frac{\alpha L}{2}$

See the transcendental equation as we found for bound states in this well! Wow!!!