8. The Finite Well and the Periodic Potential

Read §8.2 – §8.4

Problems due

7.62 cold emission

7.63 α-decay

7.87 free particle action

7.92 WKB for particle in well

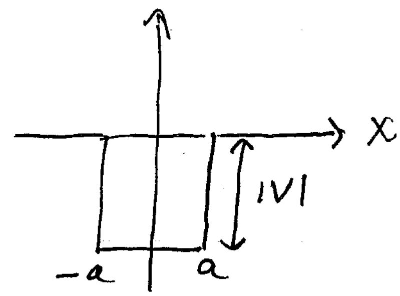
7.91

8.2 Finite Well

8.7 Semiinfinite well

8.12 periodic δ function

Finite Well

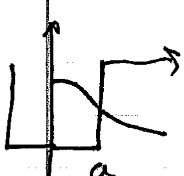


What are bound states in a rectangular potential well of finite depth?

Let the width be $2a$ and the depth be $|V|$. Because of the symmetry of the potential, we know that the eigenfunctions are either even or odd

Even soln: inside $\cos Kx$ $\qquad K^2 = \frac{2m}{\hbar^2}(|V| - |E|)$

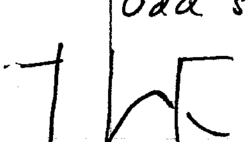
outside $e^{-\kappa x}$ $\qquad \kappa^2 = \frac{2m}{\hbar^2}|E|$



we need to match the logarithmic derivatives at the boundary $x=a$

$$\frac{-K\sin Ka}{\cos Ka} = \frac{-\kappa e^{-\kappa a}}{e^{-\kappa a}} \Rightarrow \boxed{K\tan Ka = \kappa}$$

Odd soln: inside $\sin Kx$



$$\frac{K\cos Ka}{\sin Ka} = \boxed{K\cot Ka = -\kappa}$$

These eqns determine the eigenenergies

Dimensionless variables:

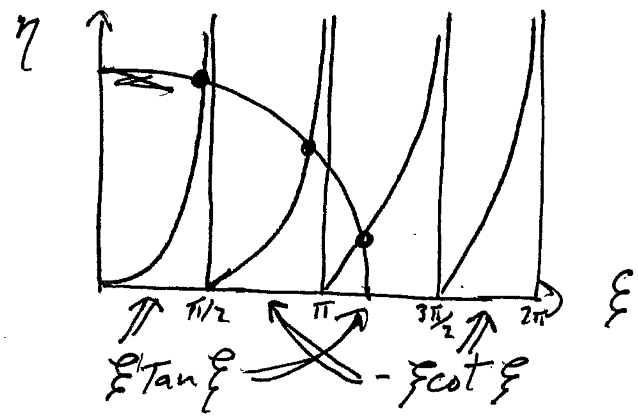
Let $\xi = ka$, $\eta = Ka$ $\Rightarrow$ $\xi^2 + \eta^2 = \frac{2m}{\hbar^2}|V|a^2 \equiv \rho^2$

("coupling constant")

Even solns $\xi \tan \xi = \eta$

Odd solns $-\xi \cot \xi = \eta$

We can imagine solving these equations graphically



Intersection of the quarter circle with the curves $\eta = \xi \tan \xi, -\xi \cot \xi$ are where bound states occur

We see that for ρ small ($\rho < \pi/2$) there is only one bound state. And each time ρ increases by $\pi/2$, another bound state "enters" the potential.

Lecture #18, 2002

Two interesting limits

- The infinite well. Let $\rho \to \infty$, and look at the most deeply bound states, i.e. the smallest values of $\xi = ka$

As radius $\to \infty$, the circle crosses that curves at $\xi = \frac{\pi}{2}, \pi, \frac{3\pi}{2}$, etc

or $ka = \frac{\pi}{2} \cdot$ integer $\Rightarrow$ $k = \frac{\pi}{2a} \cdot$ integer

– i.e. integer # of half wavelengths in the well (as seen previously)

$E - V = \hbar^2 k^2 / 2m$: energy measured from bottom of well.

• The δ function. This is the limit $a \to 0$ with $|V|2a$ fixed.

In this limit $\rho \to 0$, so we solve

$$\xi^2 + \eta^2 = \rho^2$$

$$\eta = \xi \tan \xi \sim \xi^2 \Rightarrow \eta + \eta^2 \simeq \rho^2 \text{ or } \eta \sim \rho^2$$

$$\kappa a \simeq \frac{2m}{\hbar^2}|V| a^2$$

$$\Rightarrow \kappa = \frac{2m}{\hbar^2}|V| a$$

— which does have a nonzero limit

$$= \frac{m}{\hbar^2}|V|(2a)$$

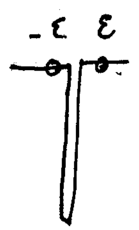
$$= \Delta$$

We can easily verify this result by solving the δ function problem directly:

Let $V(x) = \dfrac{-\hbar^2 \Delta}{m}\delta(x)$ — attractive δ-function

i.e. Schrodinger equation is

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2 \Delta}{m}\delta(x)\right]\varphi(x) = E\,\varphi(x)$$

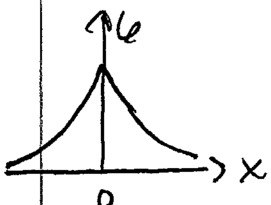


Integrate both sides $\int_{-\varepsilon}^{\varepsilon} dx$

$$\Rightarrow \frac{-\hbar^2}{2m}\left[\varphi'(\varepsilon) - \varphi'(-\varepsilon) + 2\Delta\varphi(0)\right] = 0$$

$$\Rightarrow \left.\frac{\varphi'}{\varphi}\right|_{\varepsilon} - \left.\frac{\varphi'}{\varphi}\right|_{-\varepsilon} = -2\Delta$$

i.e. -2Δ is the discontinuity in the log derivative at the origin



The bound state solution is $e^{-\kappa|x|}$ — with discontinuity -2κ in log derivative $\Rightarrow$ $\boxed{\kappa = \Delta}$

and so $K = \Delta$

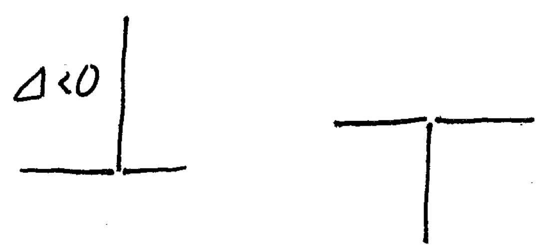
And in the δ function limit of the finite well

$$\frac{m}{\hbar^2}|U|(2a) = \Delta = K \quad \text{was found above}$$

$$\Rightarrow K^2 = \frac{2m}{\hbar^2}|E| = \Delta^2$$

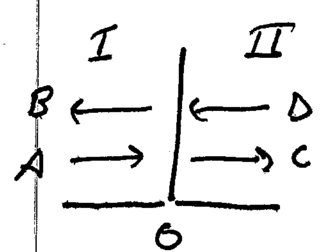
$$\text{or} \quad E = -\frac{\hbar^2}{2m}\Delta^2$$

Reflection and Transmission from δ function barrier



For $\Delta < 0$, we have a <u>repulsive</u> δ function. This is also a limit of a rectangular barrier.

But lets solve the problem from the beginning...



In fact, it is simple enough that we can solve the problem in the case where the wave in region II is not purely outgoing

$$\varphi_I = Ae^{iKx} + Be^{-iKx}$$
$$\varphi_{II} = Ce^{iKx} + De^{-iKx}$$

$\Rightarrow$ match at origin:

$$A + B = C + D$$

$$iK(A-B) = iK(C-D) + 2\Delta(A+B)$$

Eliminate D: $\quad iK(A-B) = iK(2C - A - B) + 2\Delta(A+B)$

$$\Rightarrow iK2C = iK2A - 2\Delta(A+B)$$

$$\Rightarrow \quad C = \left(1 + i\frac{\Delta}{K}\right)A + i\frac{\Delta}{K}B$$

and $\quad D = A + B - C = -i\frac{\Delta}{K}A + \left(1 - i\frac{\Delta}{K}\right)B$

Write this as a matrix:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 1+i\alpha & i\alpha \\ -i\alpha & 1-i\alpha \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \qquad \alpha = \frac{\Delta}{K}$$

(Note: we can check current conservation:

$$|C|^2 - |D|^2 = |A|^2 - |B|^2 \;)$$

This matrix has determinant $= 1$, and is easy to invert:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1-i\alpha & -i\alpha \\ i\alpha & 1+i\alpha \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

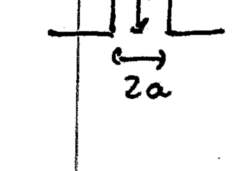
In the case where there is not incoming wave in region II, we have $D = 0 \Rightarrow$

$$\frac{A}{C} = 1 - i\alpha \qquad \frac{B}{C} = i\alpha$$

$$T' = \left|\frac{C}{A}\right|^2 = \left|\frac{1}{1-i\alpha}\right|^2 = \frac{1}{1+\alpha^2}$$

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{i\alpha}{1-i\alpha}\right|^2 = \frac{\alpha^2}{1+\alpha^2} \quad \Rightarrow \quad R + T' = 1$$

Let's check that this agrees with limiting behavior for the case of the rectangular barrier:



Consider $2a \to 0$ $\quad \frac{m}{\hbar^2} V (2a) = -\Delta$ fixed

We had found $\quad \frac{1}{T'} = 1 + \frac{V^2}{4E(V-E)} \sinh^2(K_2 2a)$

$$K_2^2 = \frac{2m}{\hbar^2}(V-E)$$

Note: the transmission amplitude

$$\frac{C}{A} = \frac{1}{1-i\alpha}$$

has a pole singularity at $\alpha = \frac{\Delta}{k} = -i$ or $k = i\Delta$

Why? Recalling that

$$\psi_I = Ae^{ikx} + Be^{-ikx} \rightarrow Ae^{-\Delta x} + Be^{\Delta x}$$

$$\psi_{II} = Ce^{-\Delta x}$$

For $\Delta > 0$,
We recognize this as the bound state solution, with $B = C$ and $A = 0$. That is C/A blows up because we have a decaying exponential in region II with no corresponding increasing exponential in region I!

A pole in the transmission amplitude, ~~and~~ at $k^2/2m = -|E_B|$ - is a general consequence of a bound state with binding energy $|E_B|$.

As $2a \to 0$ $\quad \sinh^2(K_2 2a) \simeq K_2^2(2a)^2 = \frac{2m}{\hbar^2}(V-E)(2a)^2$

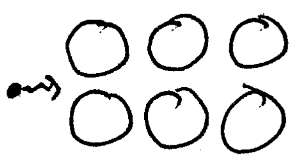
$$\Rightarrow \quad \frac{1}{T'} = 1 + \frac{V^2}{4E}\,\frac{2m}{\hbar^2}(2a)^2$$

$$= 1 + \frac{1}{2E}\,\frac{\hbar^2}{m}\Delta^2 = 1 + \frac{\Delta^2}{k^2}$$

(which does agree with $\frac{1}{T'} = 1 + \alpha^2$.)

Periodic Potential

One of the great triumphs of quantum mechanics is the theory of electrons in metals, semiconductors and insulators... How do electrons manage to move through a crystal? The atoms are packed tight... there isn't much room to squeeze through the spaces in between.



Yet somehow, in a conductor, the electrons manage to drift through... how do they do it?

The electrons don't actually squeeze through the atoms, they tunnel through. How can they tunnel through a macroscopic crystal?

For the electrons to perform this miracle, it is crucially important that the atoms