

5/15/08 Lecture 13 outline

- Particle in a finite depth box,

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

The solutions are then either even:

$$\psi_E(x) = \begin{cases} Ae^{\kappa x} & x < -a \\ B \cos kx & |x| \leq a \\ Ce^{-\kappa x} & x > a, \end{cases}$$

where $\kappa = \sqrt{2mE}/\hbar$ and $k = \sqrt{2m(V_0 - |E|)}/\hbar$, with $C = A$, or similarly for the odd solution but with \cos replaced with \sin and $C = -A$.

Note that if we write $E = K.E. + P.E.$, then the particle has positive kinetic energy in region II, $K.E. = E - V = V_0 - |E| > 0$, whereas the particle has “negative kinetic energy” in regions I and III, $K.E. = E = -|E|$. There are always oscillatory solutions where the kinetic energy is positive, and exponentially decaying solutions where the kinetic energy is negative. The above solution exhibits this general property.

The matching relation for the even solution gives

$$\kappa = k \tan(ka),$$

and the matching for the odd solutions gives

$$\kappa = -k \cot(ka).$$

There is always at least one even solution, which is the groundstate. Depending on how large $\frac{2mV_0a^2}{\hbar^2}$ is, there can be additional solutions, of increasing bound state energies, alternating between the even and odd solutions. To see how this works, consider a graphical solution of the above equations. Let $\kappa a = \eta$ and $ka = \xi$. The even matching equation can be written as

$$\eta = \xi \tan \xi, \quad \eta^2 + \xi^2 = \frac{2mV_0a^2}{\hbar^2}.$$

Plot the two equations and look for intersections of the plots. The odd solutions have

$$\eta = -\xi \cot \xi, \quad \eta^2 + \xi^2 = \frac{2mV_0a^2}{\hbar^2}.$$

There are only odd boundstates if $\frac{2mV_0a^2}{\hbar^2}$ is sufficiently large.

- In the HW you will consider exercise 5.2.2b in Shankar. Let's prove 5.2.2a: $\langle H \rangle \geq E_0$ in any state. Then show that it is possible to find a $|\psi\rangle$ such that $\langle H \rangle < 0$.

- Now let's consider the unbound solutions of the above example, with $E > 0$. Write a solution corresponding to an incoming particle, traveling to the right.

$$\psi_E(x) = \begin{cases} e^{ik_1x} + Ae^{-ik_1x} & x < -a \\ Be^{ik_2x} + Ce^{-ik_2x} & |x| \leq a \\ De^{ik_1x} & x > a, \end{cases}$$

where $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E + V_0)}/\hbar$. Matching ψ'/ψ at the boundaries yields equations for A, B, C, D . Let's first discuss some general points and work out explicitly a simpler example.

- Probability flux and conservation. We can state it in 1d, but it's more clear, and not too much more difficult, to say how it works in 3d. The 3d S.E., in position space, is

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = H\psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi.$$

It follows from this that

$$\frac{\partial}{\partial t} \rho(\vec{x}, t) + \nabla \cdot \vec{j} = 0, \quad \rho \equiv \psi^* \psi, \quad \vec{j} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*).$$

This is the statement of conservation of probability density. Classically the particle can't appear or disappear, particle number is conserved. In (non-relativistic) QM, this is a corresponding statement, that the probability a particle appears in a volume element can only change in time if there is a current flux through the surface. \vec{j} is the probability flux current density,

- Comments on delta function potential, and how the ψ' matching is affected (useful for the HW problems!): integrate the S.E. across the delta function potential to get

$$-\frac{\hbar^2}{2m} \frac{d\psi}{dx} \Big|_{x-\epsilon}^{x+\epsilon} + \int_{x-\epsilon}^{x+\epsilon} V(x)\psi(x) = 0,$$

where the second term only contributes if $V(x)$ has a delta function. Then the above equation shows that ψ' has a specific discontinuity across that x .