

Physics 521: Graduate Quantum Mechanics I

Problem Set #7 Introduction to Wave Mechanics

Best source for this subject – Merzbacher Chaps 2-8.

Due: Tuesday Oct. 21, 2014

Problem 1: Spreading of a wave packet in the Heisenberg Picture (20 points)

Consider an arbitrary free particle wave packet in 1D.

(a) Using the Heisenberg equations of motion, show

$$\frac{d}{dt}\langle\hat{x}\rangle_t = \frac{\langle\hat{p}\rangle_t}{m}, \quad \frac{d}{dt}\langle\hat{p}\rangle_t = 0,$$
$$\frac{d}{dt}\langle\hat{x}^2\rangle_t = \frac{1}{m}\langle\hat{x}\hat{p} + \hat{p}\hat{x}\rangle_t, \quad \frac{d}{dt}\langle\hat{x}\hat{p} + \hat{p}\hat{x}\rangle_t = \frac{2}{m}\langle\hat{p}^2\rangle_t$$

where the subscript means, “at time t ”.

(b) Solve these equations to find

$$\langle\hat{x}\rangle_t = \frac{\langle\hat{p}\rangle_0}{m}t, \quad \langle\hat{x}^2\rangle_t = \langle\hat{x}^2\rangle_0 + \frac{1}{m}\langle\hat{x}\hat{p} + \hat{p}\hat{x}\rangle_0t + \frac{\langle\hat{p}^2\rangle_0}{m^2}t^2$$

(c) Show that

$$\langle(\Delta\hat{x})^2\rangle_t = \langle(\Delta\hat{x})^2\rangle_0 + \frac{\langle(\Delta\hat{p})^2\rangle_0}{m^2}t^2 + \frac{2t}{m}\left(\frac{1}{2}\langle\hat{x}\hat{p} + \hat{p}\hat{x}\rangle_0 - \langle\hat{x}\rangle_0\langle\hat{p}\rangle_0\right).$$

(d) If the initial packet satisfies the minimum uncertainty product allowed by Heisenberg’s relation, and this initial distribution has no correlations between x and p , show that the packet will spread and find and sketch a graph of $\langle(\Delta\hat{x})^2\rangle_t$ vs. t .

(e) Under more general conditions the packet may initially contract and *then* spread. Use equation (c) to show how, make a sketch of the graph, and show the characteristic times.

(Aside: This is familiar in optics when a beam propagates through a focal point).

Problem 2: The Delta Function Potential in 1D (15 points).

In class we treated the case of a finite potential well of depth V_0 and width a . Suppose we take the limit $a \rightarrow 0$, $V_0 \rightarrow -\infty$, such that the product aV_0 (“area” under the potential) remains constant: $aV_0 \rightarrow U_0$. The resulting potential is a *Dirac delta function* at the origin:

$$V(x) = -U_0\delta(x): \text{(Note I have chosen the potential to be zero at infinity)}$$

(a) Using the coupled transcendental equations derived for the finite potential well, take the appropriate limit to show: there is *one* bound-state, with eigenvalue $E_0 = -\frac{mU_0^2}{2\hbar^2}$ and wave function $u_0(x) = \sqrt{\gamma} e^{-\gamma|x|}$, where $\gamma = \frac{mU_0}{\hbar^2}$. Sketch the wave function.

(b) Now solve the problem directly using the boundary conditions on the wave function across the delta function. Note, because of the singular nature, the derivative of $u(x)$ will be discontinuous. You will first need to show: $\lim_{\varepsilon \rightarrow 0} \left(\frac{\partial u}{\partial x} \Big|_{-\varepsilon} - \frac{\partial u}{\partial x} \Big|_{+\varepsilon} \right) = 2\gamma u(0)$

(c) Suppose we have a potential consisting of two delta functions, at $x = \pm b$,

$$V(x) = -U_0\delta(x-b) - U_0\delta(x+b)$$

For $b \gg 1/\gamma$, a particle bound at one delta function will not “feel” the presence of the other, and thus there are *two* almost degenerate bound eigenstates, $u_{\pm}(x) = u_0(x \pm b)$.

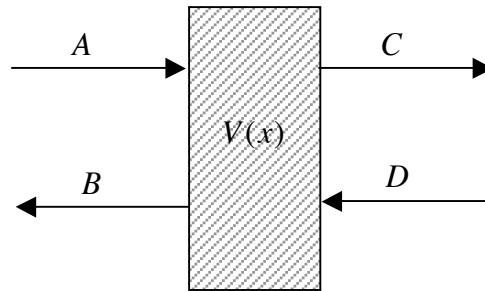
From these degenerate states, **construct** eigenstates of *parity*. Which will be the true ground state? Please sketch them

(c) If we take into account the small effect that one delta-function potential has on the wave function for a particle bound near the other, we find that the degeneracy is split, so that the difference in energy eigenvalues between the symmetric and antisymmetric eigenstates is $|E_S - E_A| = \Delta E$. Suppose at $t = 0$ the wave function is bound at one of the delta-functions, $\psi(x,0) = u_+(x)$. **Show** that the wave function oscillates, tunneling between the two delta functions with a period $T = 2\pi\hbar / \Delta E$. Give an explicit expression for $\psi(x,t)$.

(d) In the limit $b \rightarrow 0$, the two delta functions merge to make a potential $V(x) = -2U_0\delta(x)$. Knowing this, sketch a plot of the energy eigenvalues of the bound states as a function of b . Please denote the parity of the eigenstates they correspond to.

Problem 3: The S-matrix (20 points)

Consider a “localized” 1D real potential which vanishes outside some region (it may go asymptotically to zero, but we consider it to actually vanish for simplicity).



Outside the region of the potential the “scattering eigenstates” at a given energy are forward and backward propagating plane waves with amplitudes shown above. The potential relates these amplitudes. One particularly useful relation (which has important generalization to 3D scattering as we will see next semester) is the *Scattering Matrix*, known for short as the S-matrix, which relates incoming waves to outgoing waves at a fixed energy,

$$|\psi_{out}\rangle = \hat{S}|\psi_{in}\rangle \Rightarrow \begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix}$$

(a) Show that for this closed quantum system, conservation of probability implies that the S-matrix is *unitary*, and thus show, $|S_{11}| = |S_{22}|$, $|S_{12}| = |S_{21}|$, $|S_{11}|^2 + |S_{12}|^2 = 1$, $S_{11}S_{12}^* + S_{21}S_{22}^* = 0$. Argue that the eigenvalues of S are of the form $\{e^{i\phi_1}, e^{i\phi_2}\}$ with real ϕ_1, ϕ_2 known as the “scattering phase shifts”. These two parameters as a function of energy thus define all the scattering phenomenon in 1D.

For the particular case that $V(x)$ has reflection symmetry, incoming waves from the right or the left are equivalent. In that case the S-matrix takes the form,

$$S = \begin{bmatrix} r & t \\ t & r \end{bmatrix}$$

where r and t are the complex reflection and transmission *amplitudes*, with the reflection and transmission probabilities, $R \equiv |r|^2$ and $T \equiv |t|^2$. (Next Page)

(b) Using the results from (a), show that the elements of the S-matrix are defined in terms of two parameters, the amplitude and phase of the reflection coefficient,

$$r = \sqrt{R} e^{i\phi_r}, \quad t = \pm i\sqrt{1-R} e^{i\phi_r}.$$

Note: Unitarity implies the phase shift under transmission vs. reflection from a symmetric beam splitter must differ by $\pi/2$.

Relate r , t , R and ϕ_r to scattering phase shifts, ϕ_1, ϕ_2 .

(c) As an example, consider the delta-function potential from Problem 2. Show that the S-matrix is

$$S = \begin{bmatrix} r & t \\ t & r \end{bmatrix}, \quad \text{where } r = \frac{-\gamma}{\gamma + ik}, \quad t = \frac{ik}{\gamma + ik}.$$

Do these satisfy the general relations found in (a-b)?

Find the scattering phase shifts.

(d) The energy of a scattering state is $E(k) = \frac{(\hbar k)^2}{2m}$. If we analytically continue the S-matrix into the complex plane, we see that its elements have a pole at imaginary values of k . Show that that energy at this pole is none other than the bound state of the potential! This is, as we will see, a general property of the S-matrix.