Quantum Physics I (8.04) Spring 2016
Assignment 8

MIT Physics Department — *Due Friday, April 22, 2016*
April 13, 2016 — *12:00 noon*

Problem Set 8

Reading: Griffiths, pages 73-76, 81-82 (on scattering states).
Ohanian, Chapter 11: Scattering and Resonances

1. **States of the harmonic oscillator** [15 points]

   Consider the state ψ_α defined by

   $$\psi_\alpha \;\equiv\; N \exp(\alpha \hat{a}^\dagger)\, \varphi_0 \,,$$

   with $\alpha \in \mathbb{C}$ a complex number. For the first two questions below it may be helpful to simply expand the above exponential.

   (a) Find the constant N needed for the state ψ_α to be normalized.

   (b) Show that the state ψ_α is an eigenstate of the annihilation operator $\hat{a}$. What is the eigenvalue?

   (c) Find the expectation value of the Hamiltonian in the state ψ_α.

   (d) Find the uncertainty in the energy in the state ψ_α.

   (e) Use the eigenvalue equation, viewed as a differential equation to calculate the explicit form of the normalized wavefunction ψ_α.

2. **Two delta functions- again** [15 points]

   Consider again the problem of a particle of mass m moving in a one-dimensional double well potential

   $$V(x) = -g\delta(x-a) - g\delta(x+a)\,, \qquad g > 0\,.$$

   You found in the previous set the value of the bound state energy E for the even state in terms of the energy $E_0 = \hbar^2/(2ma^2)$. You had $\xi = \kappa a$

   $$\frac{E}{E_0} = -\xi^2 \qquad \text{where} \qquad \frac{\xi}{1+e^{-2\xi}} = \lambda\,, \qquad \lambda \equiv \frac{mag}{\hbar^2}\,,$$

   with λ unit free, encoding the intensity g of the delta functions, if a is constant, or the separation of the delta functions, if g is constant. We can thus write

   $$\lambda = \frac{a}{a_0} \quad a_0 \equiv \frac{\hbar^2}{mg}\,,$$

with a_0 a natural length scale in the problem once g is fixed. Introduce also the energy E_∞ associated with a single delta function:

$$E_\infty \equiv \frac{mg^2}{2\hbar^2}\,.$$

Assume now that this is a model for a diatomic molecule with interatomic distance $2a$. The bound state electron helps overcome the repulsive energy between the ions. Let the repulsive potential energy $V_r(x)$, with x the *distance* between the atoms, be given by

$$V_r(x) = \frac{\beta g}{x}\,, \quad \beta > 0\,,$$

where β is a small number. The total potential energy V_{tot} of the configuration is the sum of the negative energy E of the bound state and the positive repulsive energy:

$$V_{tot} = E + V_r(2a)\,.$$

(a) Write E as $E = -E_\infty f(\xi, \lambda)$ where f is a function you should determine. Plot E as a function of $a/a_0 = \lambda$ in order to understand how the ground state energy varies as a function of the separation between the molecules. What are the values of E for $a \to 0$ and for $a \to \infty$?

(b) Write V_r in terms of E_∞, β, and λ.

(c) Now consider the total potential energy V_{tot} and plot it as a function of $a/a_0 = \lambda$ for various values of β. You should find a critical stable point for the potential for sufficiently small β. For $\beta = 0.31$ what is the approximate value of a/a_0 at the critical point of the potential?

3. **Finite square well turning into the infinite square well** [5 points]

Consider the standard square well potential

$$V(x) = \begin{cases} -V_0\,, & \text{for } |x| \le a, \quad V_0 > 0\,, \\ 0 & \text{for } |x| > a\,, \end{cases} \tag{1}$$

and the wavefunction for an even state

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{a}}\cos kx\,, & \text{for } |x| \le a, \\ \frac{A}{\sqrt{a}} e^{-\kappa|x|}\,, & \text{for } x > |a|\,, \end{cases} \tag{2}$$

where we included the $\frac{1}{\sqrt{a}}$ prefactor to have consistent units for ψ.

We want to have a better understanding of the limit as $V_0 \to \infty$ and understand why the discontinuity in ψ' in the infinite well does not give trouble. Keeping m and a constant as we let V_0 grow large is the same as letting z_0 grow large.

A previous analysis has demonstrated that for the ground state, in the situation of large z_0, the ansatz (2) is accurately normalized and

$$\eta = ka \simeq \tfrac{\pi}{2}\left(1 - \tfrac{1}{z_0}\right), \quad \xi = \kappa a \simeq z_0\,, \qquad A \simeq \tfrac{\pi}{2z_0} e^{z_0}\,.$$

We want to see if the expectation value of the Hamiltonian receives a singular contribution from the forbidden region. Since the potential $V(x)$ vanishes there, we only need to concern ourselves with the contribution from the kinetic energy operator $\hat{K} = \frac{\hat{p}^2}{2m}$. Calculate the contribution to the expectation of $\hat{K}$ from the forbidden region $x > a$

$$\langle \hat{K} \rangle \Big|_{x>a} \equiv \int_a^\infty dx\, \psi^*(x) \hat{K} \psi(x)$$

The answer should be in terms of z_0. Interpret your result.

4. **Reflection of a wavepacket off a step potential** [20 points]

Consider a step potential with step height V_0:

$$V(x) = \begin{cases} V_0\,, & \text{for } x > 0 \\ 0\,, & \text{for } x < 0\,. \end{cases} \tag{1}$$

We send in from $x = -\infty$ a wavepacket all of whose momentum components have energies less than the energy V_0 of the step. For this we need modes with k satisfying

$$k \leq \hat{k}\,, \quad \hat{k}^2 = \frac{2mV_0}{\hbar^2}\,. \tag{2}$$

We will then write the incident wavepacket as

$$\Psi_{inc}(x) = \sqrt{a} \int_0^{\hat{k}} dk\, \Phi(k)\, e^{ikx} e^{-iE(k)t/\hbar}\,, \quad x < 0\,. \tag{3}$$

Here a is the constant with units of length, uniquely determined by the constants $m, V_0, \hbar$ in this problem, and $\Phi(k)$ is a real, unit-free function peaked at $k_0 < \hat{k}$

$$a \equiv \frac{\hbar}{\sqrt{mV_0}}\,, \quad \Phi(k) = e^{-\beta^2 a^2 (k-k_0)^2}\,. \tag{4}$$

The real constant β, to be fixed below, controls the width of the momentum distribution. The units of Ψ_{inc} are $L^{-1/2}$ and that's why we included the $\sqrt{a}$ prefactor in (3). Recall that dk has units of L^{-1}.

(a) Write the reflected wavefunction (valid for $x < 0$) as an integral similar to (3). This integral involves the phase shift $\delta(E)$ calculated in class.

Introduce a unit free version K of the wavenumber k, a unit-free version u of the coordinate x, and a unit-free version τ of the time t as follows

$$k \equiv \frac{K}{a}\,, \quad x \equiv au\,, \quad t \equiv \frac{\hbar}{V_0}\,\tau\,. \tag{5}$$

Naturally, we will write $k_0 = K_0/a$. Note that $kx = Ku$.

(b) Show that the group velocity and the uncertainty relation for the incoming packet take the form

$$\frac{du}{d\tau} = \#K_0\,, \qquad \Delta u\,\Delta K \geq \#\,,$$

where # represent *numerical* constants that you should fix (different constants!). Use the approximation that we have the full gaussian $|\Phi(K)|^2$ to determine the uncertainty ΔK in the incoming packet in terms of β. Assuming again that we have a full gaussian, what would be (in terms of β) the minimum possible value of the uncertainty Δu for the associated coordinate space probability distribution?

(c) Complete the following equations by fixing the constants represented by #

$$E(k) = \#V_0K^2\,, \quad e^{2i\delta(E)} = \# + \#K^2 + iK\sqrt{\# + \#K^2} \equiv w(K)\,.$$

(d) Show that the delay $\Delta t = 2\hbar\,\delta'(E)$ experienced by the reflected wave implies a $\Delta\tau$ given by

$$\Delta\tau = \frac{\#}{K_0\sqrt{\# + \#K_0^2}}\,,$$

where you must fix the constants.

(e) Prove that the complete wavefunction $\Psi(x,t)$ valid for $x < 0$ and all times, which we now view as $\Psi(u,\tau)$ valid for $u < 0$ and all τ, takes the form

$$a^{\frac{1}{2}}\Psi(u,\tau) = \int_0^{\#} dK e^{-\beta^2(K-K_0)^2} e^{-i\#K^2\tau}\left(e^{iKu} - e^{-iKu}w(K)\right)$$

and determine the two missing constants.

(f) Set $\beta = 4$ and $K_0 = 1$. What are the values of ΔK and Δu? What is the predicted time delay $\Delta\tau$? (Not graded: Can you make an informed guess if the packet will change shape quickly?)

Now use Mathematica to calculate and make plots of the probability density $|a^{\frac{1}{2}}\Psi(u,\tau)|^2$. Give the plot of the wavefunction for $\tau = -20, -5$, and 0, and using $u \in [-30, 0]$. Examine the plot for $\tau = 20$ and determine the time delay $\Delta\tau$ by looking at the position of the peak of the packet. Your answer should come reasonably close to the analytical value you determined previously.

5. **Scattering off a rectangular barrier.** Based on Griffiths 2.33. p.83. [10 points]

Do only the cases $E < V_0$ and $E = V_0$.

Can you get $T = 1$ for $E < V_0$?

Find the answer for $E > V_0$ in some book (or do it). When does one get $T = 1$ for $E > V_0$?

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