Homework 4

PHYS 485: Fall 2017
Due Date: 10/18/2017

To recieve fully credit please write legibly and clearly, show all required steps and calculations and answer any explicit questions in full sentences.

I. REFRESHER: CALCULATING EIGENVALUES AND EIGENVECTORS OF MATRICES [8]

Consider a system of 2 coupled linear equations

$$\begin{aligned} 3x + 4y &= \alpha x \\ 4x - 1y &= \alpha y \end{aligned} \tag{1}$$

(a) Re-write this system as a matrix-based relationship in the x, y basis. In particular, find a 2×2 matrix M such that $M\vec{r} = \alpha\vec{r}$ for $\vec{r} = \begin{pmatrix} x \\ y \end{pmatrix}$. [1]

(b) Find the two eigenvalues α_1 and α_2 of the matrix M by solving the determinant equation [2]

$$\begin{vmatrix} 3-\alpha & 4 \\ 4 & -1-\alpha \end{vmatrix} = 0.$$

(c) For each of the two eigenvalues that you found, find the relationship between x and y that satifies Eq. (1). Namely, find β_1 and β_2 such that $y = \beta_1 x$ and $y = \beta_2 x$ for α_1 and α_2, respectively. [2]

(d) Now, the following vector is an eigenvector of M:

$$\vec{v}_1 = \begin{pmatrix} x \\ \beta_1 x \end{pmatrix}, \tag{2}$$

and similarly for $\vec{v}_2$. In both cases, find x by requiring that $\vec{v}_i$ be normalized: $\vec{v}_1 \cdot \vec{v}_1 = 1$ and $\vec{v}_2 \cdot \vec{v}_2 = 1$. [2]

(e) Show that the eigenvectors $\vec{v}_1$ and $\vec{v}_2$ are orthogonal i.e. that their dot product vanishes. This result, combined with enforcing $\vec{v}_1 \cdot \vec{v}_1 = 1$ ($\vec{v}_2 \cdot \vec{v}_2 = 1$) in the previous part of the problem, shows that $\vec{v}_1$ and $\vec{v}_2$ form an orthonormal basis. [1]

II. DOUBLE WELL POTENTIAL AND TUNNELING [12]

Consider an electron in the double potential well shown in Fig. 1.

(a) Draw the ground state wavefunction, ψ_R (right) and ψ_L (left), for each of the potential wells in Fig. 1 (a). Assume that the state described by ψ_R has energy E_R and the state described by ψ_L has energy E_L. [2]

(b) Now, suppose that the barrier between the two wells is large (much larger than E_L and E_R) but finite and of height V_0 as shown in Fig. 1 (b). Draw the wavefunctions for the ground state and the first excited state of this combined system. [2]

(c) To find the energies of eigenstates you have drawn above, we can use the formalism of Problem I. More precisely, we can write the Hamiltonian of the combined system as a matrix in the (ψ_R, ψ_L) basis where ψ_L can be denoted by $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and ψ_R can be taken to be equal to $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In this basis, the Hamiltonian of the combined system reads:

$$H = \begin{pmatrix} E_R & t \\ t & E_L \end{pmatrix}$$

where t is the strength for tunneling through the large barrier. Following the procedure you used to find the eigenvalues and eigenvectors of M in Problem I, find the same quantities for H. [4]

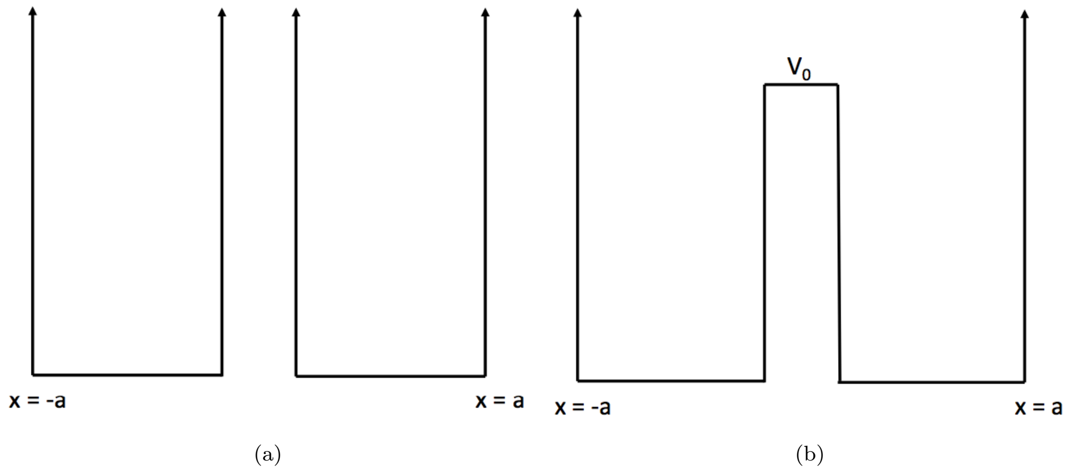

FIG. 1: Double potential well discussed in Problem II.

(d) For the eigenvector corresponding to the lower energy state (smaller eigenvalue), what is the probability of the electron being described by ψ_R? What is the probability of the electron being described by ψ_L? [2]

(e) Suppose an electron is in the ground state of this system and gets excited to the first excited state by absorbing a photon. What is the wavelength of this photon in terms of E_R, E_L, t and fundamental constants? [2]

III. LENNARD-JONES POTENTIAL [8]

The Lennard-Jones potential is a simple model commonly used to approximate interactions (for instance van der Waals) between pairs of particles at the atomic scale. It is given by:

$$V_{\rm LJ}(r) = V\left(\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right).$$

Here, r is the distance between the atoms. For small displacement (δr) of atoms away from the equilibrium position, this system of particles acts as a spring in that $V_{\rm LJ}$ exerts a restoring force such that $V(r) \approx V_0 + \frac{1}{2}k(\delta r)^2$. Here you will find the spring constant k by Taylor expanding $V_{\rm LJ}$.

(a) Sketch the Lennard-Jones potential [1]

(b) (i) Determine the value of $r = r_{\rm min}$ such that $V(r)$ is minimized. *Hint: Consider finding an r such that* $\frac{\partial V_{\rm LJ}}{\partial r}|_{r=r_{\rm min}} = 0$.

(ii) Use $r_{\rm min}$ to find V_0 in terms of r_0 and V. [2]

(c) Calculate the value of the second derivative of $V_{\rm LJ}(r)$ at the minimum value of the potential i.e. at $r_{\rm min}$. [1]

(d) Find the angular frequency of oscillation about $r_{\rm min}$ by recalling that $\omega = \sqrt{k/m}$ and the spring constant k is related to the second derivative you have calculated above. Here, m is the effective mass of the two particles combined. [2]

(e) Treating this oscillation quantum mechanically, what is the energy difference between the ground state and the first excited state? Give the value of this energy in electronvolts for $r_0 = 0.34$ nm and $V = 9.949$ meV. [2]

IV. QUANTUM HARMONIC OSCILLATOR [12]

Consider a quantum harmonic oscillator of mass m having a spring constant k.

(a) (i) Explicitly write down the normalized ground state wavefunction, ψ_0, and the wavefunctions, ψ_1, ψ_2, of the first two excited states for this system.

(ii) What are the energies of these states?

(iii) Sketch the potential and these wavefunctions on the same plot and label them clearly. [3]

(b) Now suppose the oscillator is prepared in a superposition state, $\Psi(x, t = 0)$, of the first excited state and the second excited state with equal amplitudes at $t = 0$. What is $\Psi(x, t)$ in terms of ψ_1 and ψ_2 and their energies i.e how does this state evolve in time? Make sure to normalize $\Psi(x, t)$ as appropriate. [2]

(c) Calculate $\langle E \rangle$ for $\Psi(x, t)$. Does it depend on time? Explain. [2] *Hint: No complicated calculations are necessary in this part of the problem.*

(d) Calculate and plot $\langle x(t) \rangle$ for . How does it compare to the classical harmonic operator? Discuss. [5]
Hint: To evaluate the integrals in this problem you will need to use the following identities:

$$\int_{-\infty}^{\infty} f(x)dx = 0 \text{ for any even function f(x) = f(−x),}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\beta x^2} dx = \frac{1}{2\beta}\sqrt{\frac{\pi}{\beta}},$$

$$\int_{-\infty}^{\infty} x^4 e^{-\beta x^2} dx = \frac{3}{4\beta^2}\sqrt{\frac{\pi}{\beta}}.$$