AQM Problem Set 0 (Review)

Problem 1: Solve the Schrödinger equation (i.e. find the eigenvalues and eigenstates, then plot typical eigenstates) with the following 1D Hamiltonians

$$H = \frac{p^2}{2m} + V(x),$$

where

$$(a) V(x) = \frac{1}{2} m\omega^2 x^2;$$
$$(b) V(x) = V_0 \theta(L/2 - |x|) \text{ with } \theta(x) \text{ the Heaviside step function;}$$
$$(c) V(x) = V_0 \left[\delta(x + L/2) + \delta(x - L/2)\right] \text{ with } \delta(x) \text{ the Dirac delta function.}$$

Problem 2: Describe the following experiments (drawing pictures is recom- mended) and interpret the observations:

(a) double-slit experiment with single particles (e.g. photons, electrons, atoms, molecules, etc.);
(b) Stern-Gerlach experiment;
(c) Aharonov-Bohm effect.

Problem 3 (optional): Solve the hydrogen atom model:

$$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

**Drafted by me and revised by GPT-4o.*

Answer 1:

(a) For a harmonic oscillator, the eigenvalues and eigenstates can be obtained by introducing the phonon annihilation operator ($\hat{b}$) and creation operator ($\hat{b}^\dagger$):

$$\begin{aligned}\hat{b} &= \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega\hat{x}),\\ \hat{b}^\dagger &= \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega\hat{x}),\end{aligned} \tag{1}$$

which satisfy $[\hat{b}, \hat{b}^\dagger] = 1$. Then the Hamiltonian can be rewritten as:

$$\hat{H} = \hbar\omega(\hat{b}^\dagger\hat{b} + \frac{1}{2}). \tag{2}$$

We can see that the energy of the system will increase if we apply the creation operator to the system. We will demonstrate this by using the operator $\hat{H}$ to find the new energy of the system (assuming $\hat{H}\psi = E\psi$):

$$\begin{aligned}\hat{H}(\hat{b}^\dagger\psi) &= \hbar\omega(\hat{b}^\dagger\hat{b}\hat{b}^\dagger + \frac{1}{2}\hat{b}^\dagger)\psi\\ &= \hbar\omega(\hat{b}^\dagger(\hat{b}\hat{b}^\dagger) + \frac{1}{2}\hat{b}^\dagger)\psi\\ &= \hbar\omega(\hat{b}^\dagger(\hat{b}^\dagger\hat{b} + 1) + \frac{1}{2}\hat{b}^\dagger)\psi\\ &= \hat{b}^\dagger(\hat{H} + \hbar\omega)\psi\\ &= (E + \hbar\omega)(\hat{b}^\dagger\psi).\end{aligned} \tag{3}$$

Similarly, $\hat{H}(\hat{b}\psi) = (E - \hbar\omega)(\hat{b}\psi)$. Since a state with energy lower than the ground state does not exist, the lowest energy state satisfies

$$\hat{b}\psi_0 = 0. \tag{4}$$

Based on Eq. (4), we can derive the eigenenergy of the ground state:

$$\hat{H}\psi_0 = \hbar\omega(\hat{b}^\dagger\hat{b} + \frac{1}{2})\psi_0 = \frac{1}{2}\hbar\omega\psi_0. \tag{5}$$

By repeatedly applying the raising operator, we can obtain all *eigenenergies* of the oscillator:

$$\hat{H}\psi_n = \hat{H}((\hat{b}^\dagger)^n\psi_0) = \hbar\omega(n + \frac{1}{2})\psi_n, \tag{6}$$

where $n = 0, 1, 2, \ldots$ denotes the energy level. We can also obtain the differential equation for the ground eigenstate using Eq. (4):

$$\begin{aligned}\hat{b}\psi_0 &= \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega\hat{x})\psi_0\\ &= \frac{1}{\sqrt{2\hbar m\omega}}(\hbar\frac{d\psi_0}{dx} + m\omega x\psi_0) = 0.\end{aligned} \tag{7}$$

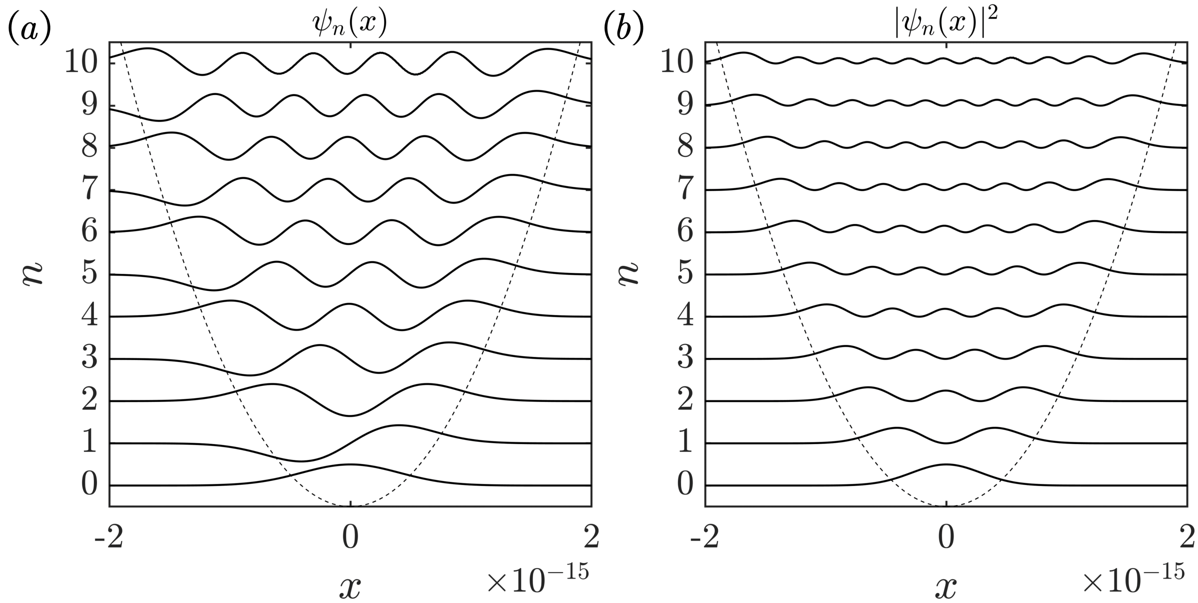

FIG. 1. (a) Eigenfunctions $\psi_n(x)$ versus position x for different energy levels n. (b) Probability distributions $|\psi_n(x)|^2$ versus x for different energy levels n. The dashed lines represent the classical limit. The parameters chosen are experimentally feasible: $m = 10$ ng, $\omega = 64 \times 10^6$ Hz.

We can solve Eq. (7) by separating variables:

$$\begin{aligned} \frac{1}{\psi_0} d\psi_0 &= -\frac{m\omega x}{\hbar} dx \\ \Rightarrow \ \ln|\psi_0| &= -\frac{m\omega x^2}{2\hbar} + C \\ \Rightarrow \ \psi_0 &= A\exp(-\frac{m\omega x^2}{2\hbar}). \end{aligned} \tag{8}$$

Here, C is a constant and $A = (\frac{m\omega}{\pi\hbar})^{1/4}$ is the normalization coefficient. From Eq. (6), we can easily derive that $\hat{b}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}$. Therefore, the *eigenfunctions* are

$$\psi_n = \frac{(\hat{b}^\dagger)^n}{\sqrt{n!}}\psi_0. \tag{9}$$

Using Eqs. (6) and (9), I plotted Figs. 1(a) and 1(b), which illustrate the wavefunction and probability distribution of the harmonic oscillator (solid lines) for different energy levels n, respectively, along with the classical limit (dashed lines). The wavefunction and probability distribution are normalized such that their maximum amplitude is 0.5. In Fig. 1(a), it is observed that the parity of the energy levels n correlates with the parity of the wavefunctions: if n is even, the wavefunctions exhibit even parity, and if n is odd, the wavefunctions exhibit odd parity. Additionally, as shown in Fig. 1(b), with the increase of the energy level n, the probability distribution approaches the classical limit, consistent with the Bohr Correspondence Principle.

(b) If $V_0 = 0$, the system is trivial. Therefore, we will consider the cases where $V_0{<}0$ & $V_0{<}E{<}0$, $V_0{<}0$ & $E{>}0$, $V_0{>}0$ & $E{<}V_0$ and $V_0{>}0$ & $E{>}V_0$.

Case I ($V_0{<}0$ & $V_0{<}E{<}0$):
If $V_0{<}0$, the system is a finite square potential well. If the energy of the particle E satisfy $V_0{<}E{<}0$, it will be the bound state. The Schrödinger equation of the system is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi. \tag{10}$$

Then we substitute the potential energy $V(x) = V_0\theta(L/2 - |x|)$ with $|x|{>}L/2$ into Eq. (10):

$$\nabla^2\psi = \beta^2\psi, \tag{11}$$

where $\beta^2 = -\frac{2mE}{\hbar^2}$. The solution of this differential equation is $\psi = C\exp(\pm\beta x)$. By using the boundary condition: $\psi(\pm\infty) = 0$, we will obtain the wavefunction:

$$\begin{aligned} \psi_{(x>L/2)} &= A\exp(-\beta x) \\ \psi_{(x<L/2)} &= B\exp(\beta x). \end{aligned} \tag{12}$$

Here, A and B are normalization coefficient. Then we consider the situation that $|x|{<}L/2$, the Schrödinger equation is:

$$\nabla^2\psi = -k^2\psi, \tag{13}$$

where $k^2 = \frac{2m(E-V)}{\hbar^2}$. The solution of this differential equation is $\psi = C_1\sin(kx)$ or $C_2\cos(kx)$,

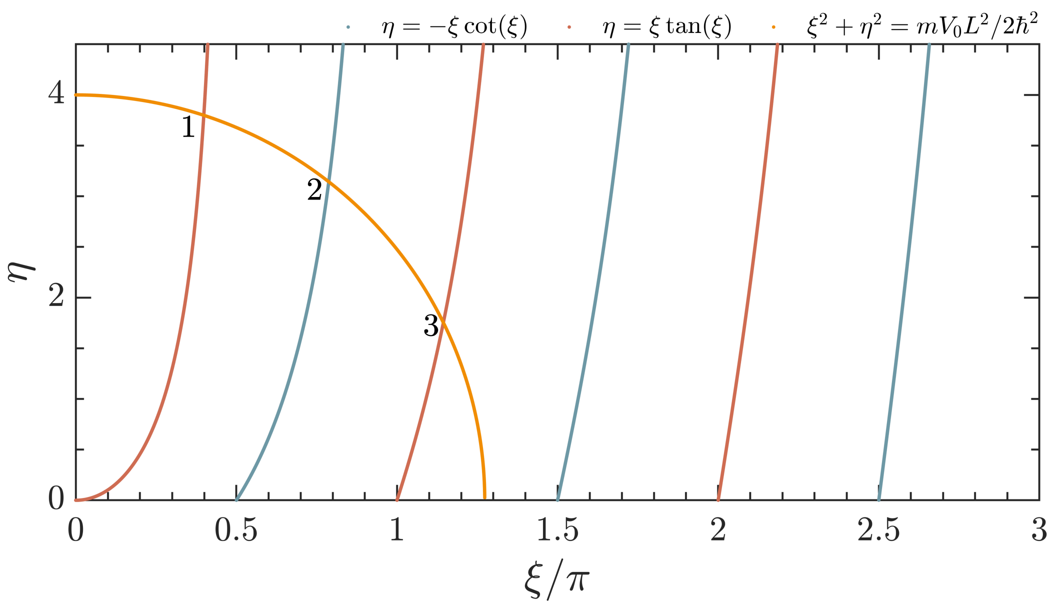

FIG. 2. The figure of Eqs. (15) and (16). The points where the yellow line intersects with the red or blue lines represent the existing energy levels. The parameters chosen are m=1kg, L=1m and $V_0 = 32\hbar^2$J.

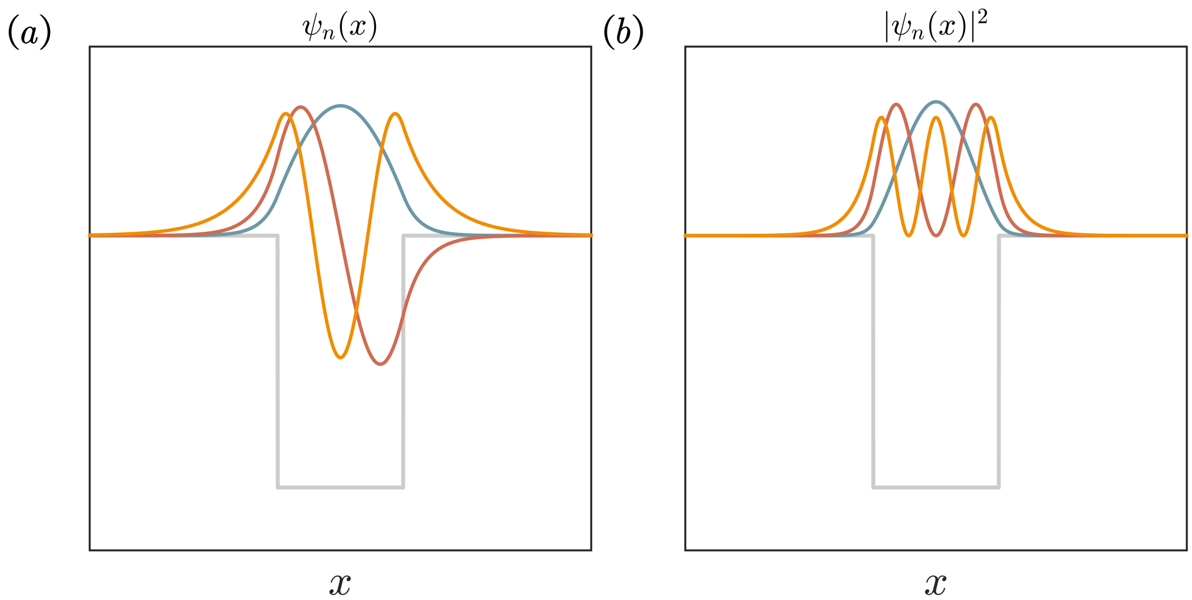

FIG. 3. (a) Eigenfunctions $\psi_n(x)$ versus position x corresponding to different regions in Fig. 2. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x for the same regions in Fig. 2. The blue, yellow, and red lines correspond to regions 1, 2, and 3, respectively, in Fig. 2, while the grey line represents the potential energy.

which is decided by the parity:

$$\begin{aligned}&\text{If the parity of state is odd,}\, \psi_{(|x|<L/2)} = C_1 \sin(kx).\\ &\text{If the parity of state is even,}\, \psi_{(|x|<L/2)} = C_2 \cos(kx).\end{aligned} \tag{14}$$

By using the boundary condition: $\psi(\frac{L}{2}^+) = \psi(\frac{L}{2}^-)$ and $\psi(-\frac{L}{2}^+) = \psi(-\frac{L}{2}^-)$, and $\ln(\dot{\psi})$ exhibits similar behavior, we have:

$$\begin{aligned}-\xi \cot \xi &= \eta, \ \text{(odd parity)}\\ \xi \tan \xi &= \eta, \ \text{(even parity).}\end{aligned} \tag{15}$$

Here, $\xi = \frac{kL}{2}$, $\eta = \frac{\beta L}{2}$. Additionally, from the definitions of ξ and η, we have

$$\xi^2 + \eta^2 = \frac{mV_0L^2}{2\hbar^2}. \tag{16}$$

Based on Eqs. (15) and (16), I plotted Fig. (2), the points where the yellow line intersects with the red or blue lines represent the existing energy levels.
Figure 3 show the eigrnfunctions and probability distributions based on Eqs. (12) and (14).