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 satisfies $[\hat{b}, \hat{b}^\dagger] = 1$. 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 no state with energy lower than the ground state exists, 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 as:

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

By repeatedly applying the raising operator, we can obtain all the *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):

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

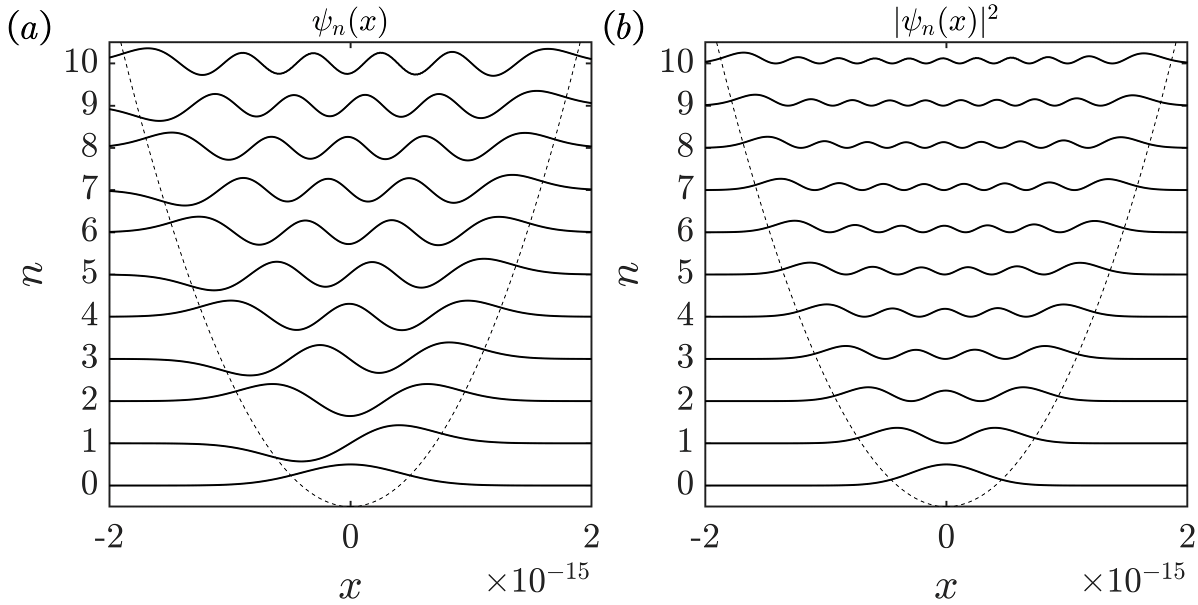

FIG. 1. (a) Eigenfunctions $\psi_n(x)$ versus position x for different energy levels n. (b) Probability distributions $|\psi_n(x)|^2$ versus x for different energy levels n. The dashed lines represent the classical limit. The chosen parameters are experimentally feasible: $m = 10$ ng, $\omega = 64 \times 10^6$ 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), as the energy level n increases, the probability distribution approaches the classical limit, consistent with the Bohr Correspondence Principle.

(b) If $V_0 = 0$, the system is trivial. If $E \leq \min(V)$, the situation is physical unfeasible. Therefore, we will consider the cases where $V_0{<}0$ & $V_0{<}E{<}0$, $V_0{<}0$ & $E{>}0$, $V_0{>}0$ & $0{<}E{<}V_0$ 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:

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

We then substitute the potential energy $V(x) = V_0\theta(L/2 - |x|)$ for $|x|{>}L/2$ 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 coefficients. Then we consider the situation that $|x|{<}L/2$, the Schrödinger equation is:

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

where $k^2 = \frac{2m(E-V_0)}{\hbar^2}$. The solution of this differential equation is $\psi = C_1\sin(kx)$ or $C_2\cos(kx)$,

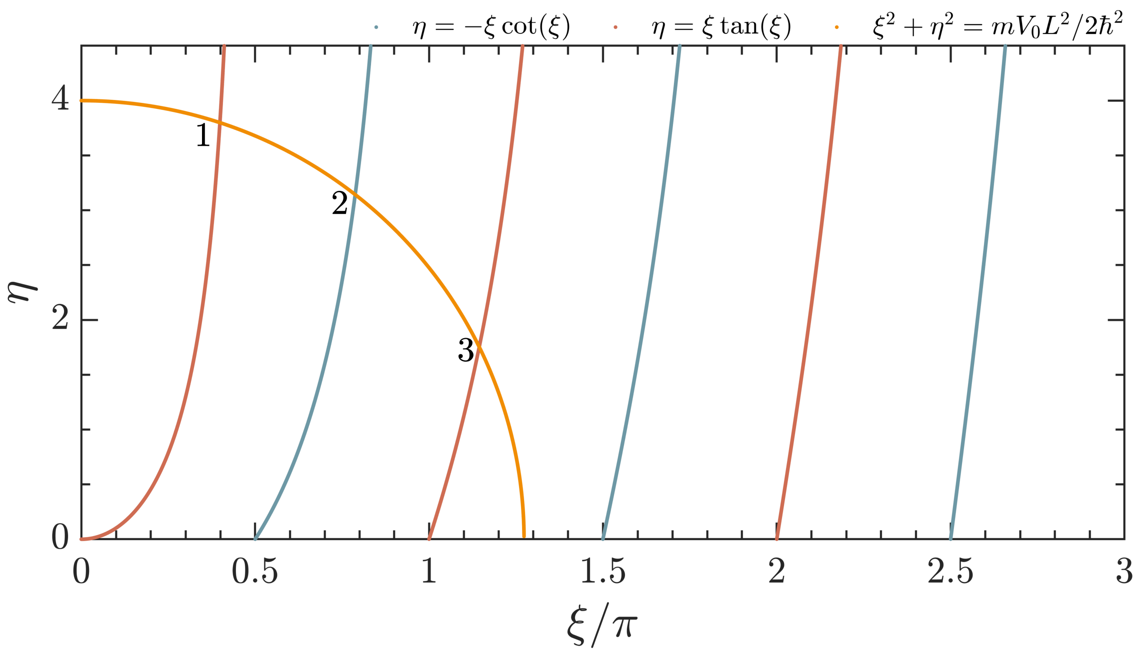

FIG. 2. The figure of Eqs. (15) and (16). The points where the yellow line intersects with the red or blue lines represent the existing energy levels. The parameters chosen are m=1kg, L=1m and $V_0 = -32\hbar^2$J.

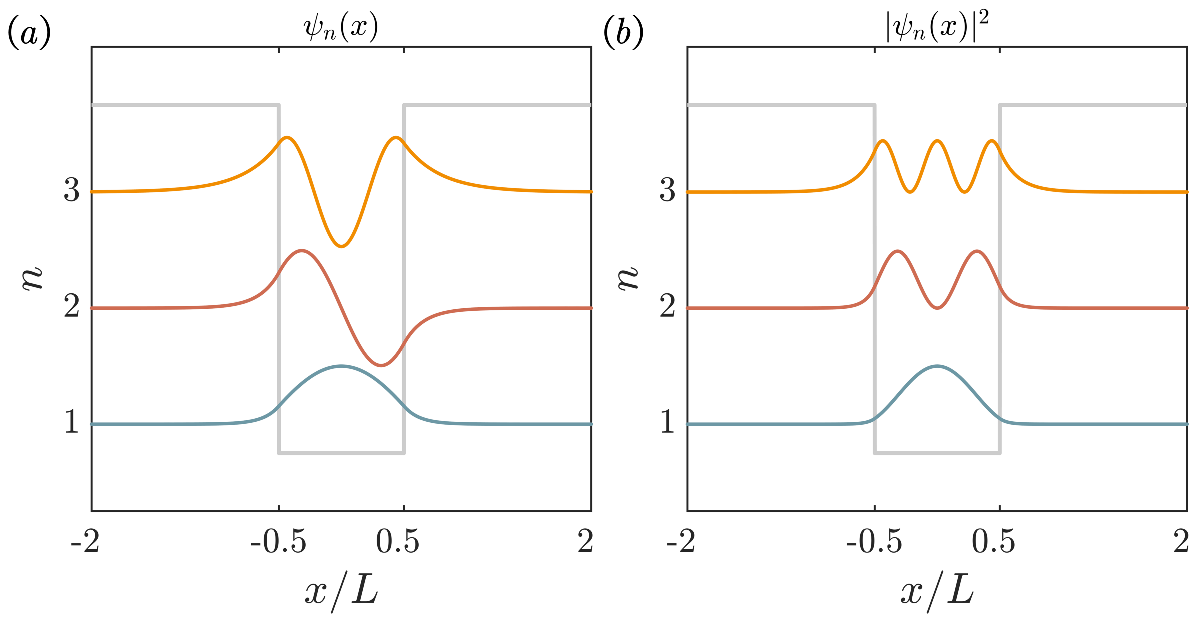

FIG. 3. (a) Eigenfunctions $\psi_n(x)$ versus position x corresponding to different regions in Fig. 2. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x for the same regions in Fig. 2. The blue, yellow, and red lines correspond to regions 1, 2, and 3, respectively, in Fig. 2, while the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

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).
In conclusion, in this case, the *eigenenergy* of the system is $E = -2\hbar^2\eta_n^2/mL^2$. The *eigenfunction* of the system is

$$\begin{aligned}&\psi_{(x>L/2)} = A\exp(-\beta x), && \psi_{(x<L/2)} = B\exp(\beta x),\\ &\psi_{(|x|<L/2)} = C_1 \sin(kx), \ \text{n is odd}, && \psi_{(|x|<L/2)} = C_2 \cos(kx), \ \text{n is even}.\end{aligned} \tag{17}$$

Case II (V_0<0 & E>0):
For this case, the energy of the particle is greater than the maximum energy of the potential. However, in Quantum work, the spread of the particle is also affected by the potential well. The energies are continue and We assume the particle is spread along the x-axis and initially located on the left side of the potential well. The Schrödinger equation with $|x|>L/2$ is:

$$\nabla_x \psi = -k^2 \psi, \tag{18}$$

where $k = \sqrt{2mE}/\hbar$. By considering the input direction, we can obtain the corresponding solutions:

$$\begin{aligned} \psi_{(x<-L/2)} &= A\exp(ikx) + rA\exp(-ikx), \\ \psi_{(x>L/2)} &= tA\exp(ikx). \end{aligned} \tag{19}$$

Here, A ,r and t are coefficients. Because the state is continuous, we can't normalize the wave function, so the coefficient A is not very important. What we care about is the relative impact from the energy well, which is reflected by r and t. These are related to the reflection rate and transmission rate, respectively.
When $|x|<L/2$, the Schrödinger equation is

$$\nabla_x \psi = -k'^2 \psi, \tag{20}$$

where $k' = \sqrt{2m(E - V_0)}/\hbar$. The solution is

$$\psi_{(|x|<L/2)} = B\exp(ik'x) + C\exp(-ik'x). \tag{21}$$

Due to the wavefunctions and it's derivatives for this case are continue, we have these functions (Here, we set $B = bA$, $C = cA$, and $x \to x + L/2$ to simplify the calculation, and we have to make $x \to x - L/2$ after obtaining the wavefunctions):

$$1 + r = b + c \tag{22a}$$

$$\frac{k}{k'}(1 - r) = b - c \tag{22b}$$

$$t\exp(ikL) = b\exp(ik'L) + c\exp(-ik'L) \tag{22c}$$

$$\frac{k}{k'}t\exp(ikL) = b\exp(ik'L) - c\exp(-ik'L). \tag{22d}$$

From Eqs. (22a) and (22b), we can obtain b and c:

$$\begin{aligned} b &= \frac{1}{2}\left[(1 + \frac{k}{k'}) + r(1 - \frac{k}{k'})\right], \\ c &= \frac{1}{2}\left[(1 - \frac{k}{k'}) + r(1 + \frac{k}{k'})\right]. \end{aligned} \tag{23}$$

Based on Eqs. (22c) and (22d), we can also obtain b and c:

$$\begin{aligned} b &= \frac{t}{2}(1 + \frac{k}{k'})\exp(ikL - ik'L), \\ c &= \frac{t}{2}(1 - \frac{k}{k'})\exp(ikL + ik'L). \end{aligned} \tag{24}$$

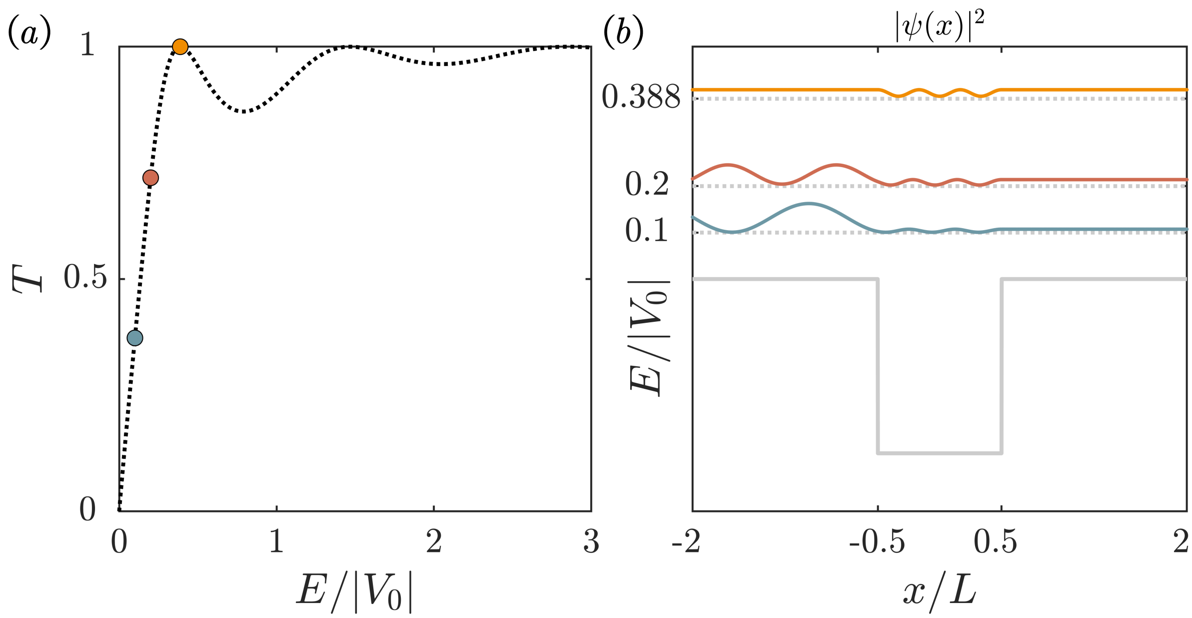

FIG. 4. (a) The transmission versus the energy of the particle $E/|V_0|$. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x/L with different the energy of the particle. The dots in (a) are corresponding with the lines in (b) with same color. The parameters are the same as in Fig. (2).

Substituting Eq. (23) into Eq. (24):

$$
\begin{aligned}
&(1+\frac{k}{k'})+r(1-\frac{k}{k'})=t(1+\frac{k}{k'})\exp(ikL-ik'L),\\
&(1-\frac{k}{k'})+r(1+\frac{k}{k'})=t(1-\frac{k}{k'})\exp(ikL+ik'L).
\end{aligned}
\tag{25}
$$

Then we can solve t and r:

$$
\begin{aligned}
t&=\frac{-2k/k'\cdot\exp(-ikL)}{[1-(k/ik')^2]\sinh(ik'L)-2(k/k')\cosh(ik'L)}=\frac{\exp(-ikL)}{\cos(k'L)-\frac{i}{2}(\frac{k}{k'}+\frac{k'}{k})\sin(k'L)},\\
r&=\frac{-\frac{1}{2}\left(\frac{k}{k'}-\frac{k'}{k}\right)\sinh(ik'L)}{\cosh(ik'L)+\frac{1}{2}\left(\frac{k}{k'}+\frac{k'}{k}\right)\sinh(ik'L)}=\frac{-\frac{i}{2}\left(\frac{k}{k'}-\frac{k'}{k}\right)\sin(k'L)}{\cos(k'L)-\frac{i}{2}\left(\frac{k}{k'}+\frac{k'}{k}\right)\sin(k'L)}.
\end{aligned}
\tag{26}
$$

As we know, the probability current density in quantum mechanics is

$$
j=\frac{\hbar}{2mi}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\nabla\psi\right).
\tag{27}
$$

For the input wave, $j_{in}=\frac{\hbar k}{m}=|A|^2v$. or the reflection part of $\psi_{(x<-L/2)}$, $j_r=|r|^2|A|^2v$, for the transmission wave $(\psi_{(x>-L/2)})$, $j_t=|t|^2|A|^2v$. So the reflection rate is

$$
R=j_r/j_{in}=|r|^2,
\tag{28}
$$

the transmission rate is

$$
T=j_t/j_{in}=|t|^2.
\tag{29}
$$

In Fig. (4), we can see that the transmission rate $T=1$ when $k'L=n\pi, n=1,2,3,\cdots$, which is called resonant transmission.

Case III (V_0>0 & 0<E<V_0):
For this case, the solution is similar with case II. We also can make $ik' \to \kappa$, where $\kappa = \sqrt{-2m(E-V_0)}/\hbar$, and then the form of the solution will be the same as in the textbook:

$$t = \frac{-2ik/\kappa \cdot \exp(-ikL)}{[1-(k/\kappa)^2]\sinh(\kappa L) - 2i(k/\kappa)\cosh(\kappa L)},$$
$$r = \frac{-\frac{i}{2}\left(\frac{k}{\kappa}+\frac{\kappa}{k}\right)\sinh(\kappa L)}{\cosh(\kappa L)+\frac{i}{2}\left(\frac{k}{\kappa}-\frac{\kappa}{k}\right)\sinh(\kappa L)}. \tag{30}$$

The wave function with $|x|<L/2$ is

$$\psi_{(|x|<L/2)} = B\exp(\kappa x) + C\exp(-\kappa x). \tag{31}$$

Figure 5 show the transmission rate and the wavefunction for this case. We can find that even though the particle's energy is lower than the energy barrier, the particle still has a probability of tunneling through the barrier, as I have shown in Figs. 5(a) and 5(b), which is called the tunneling effect, and it is a kind of quantum effect that does not exist in classical physics.
By decreasing the mass of the particle, the tunneling effect will become more pronounced, as I shown in Figs. 6(a) and 6(b).

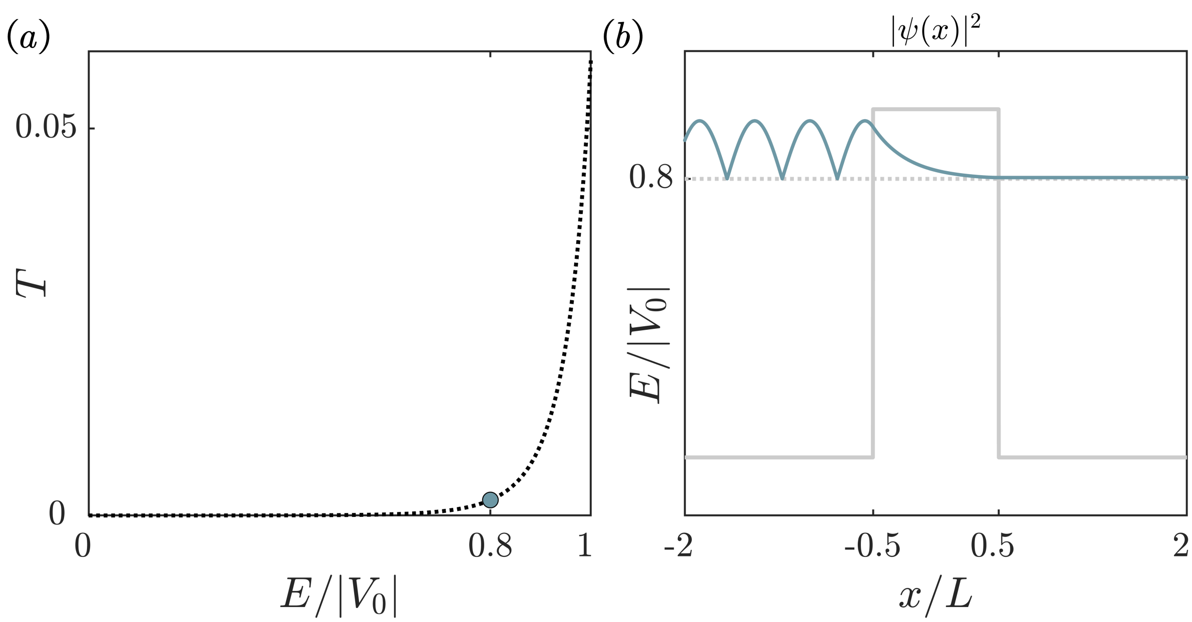

FIG. 5. (a) The transmission versus the energy of the particle $E/|V_0|$. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x/L with different the energy of the particle. The dots in (a) are corresponding with the lines in (b) with same color. $V_0 = 32\hbar^2$J, the other parameters are the same as in Fig. (2).

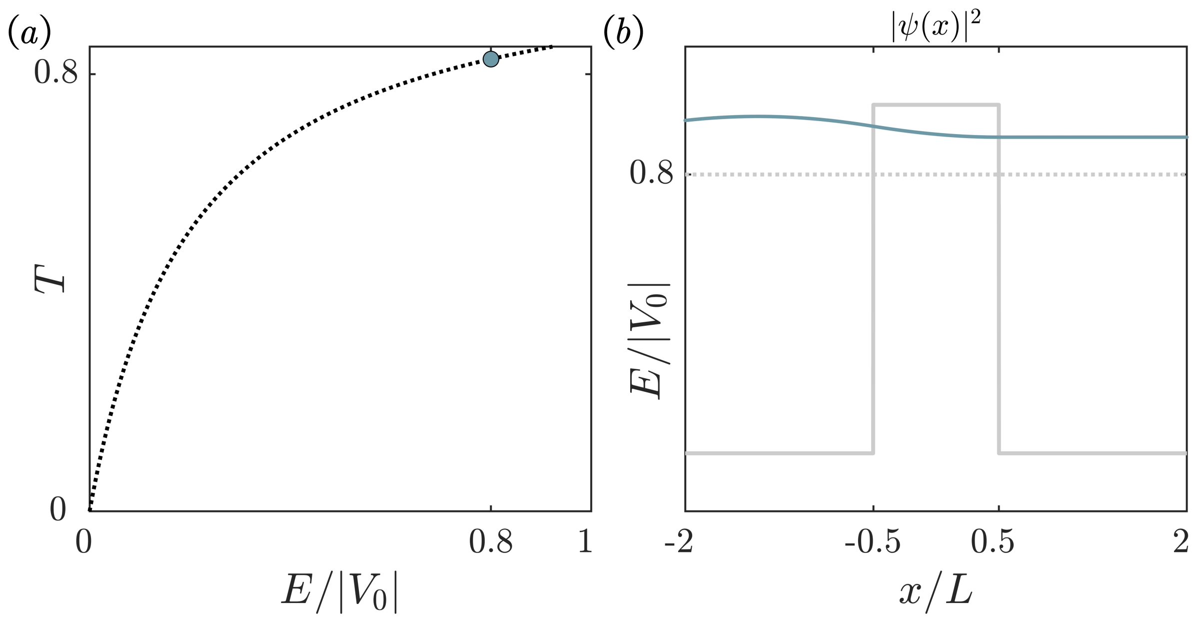

FIG. 6. (a) The transmission versus the energy of the particle $E/|V_0|$. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x/L with different the energy of the particle. The dots in (a) are corresponding with the lines in (b) with same color. $V_0 = 32\hbar^2$J and $m = 0.01$kg, the other parameters are the same as in Fig. (2).

Case IV (V_0>0 & E>V_0):
For this case, the solution is same with case III and the physics is quite like case II, as I shown in Fig. (7).

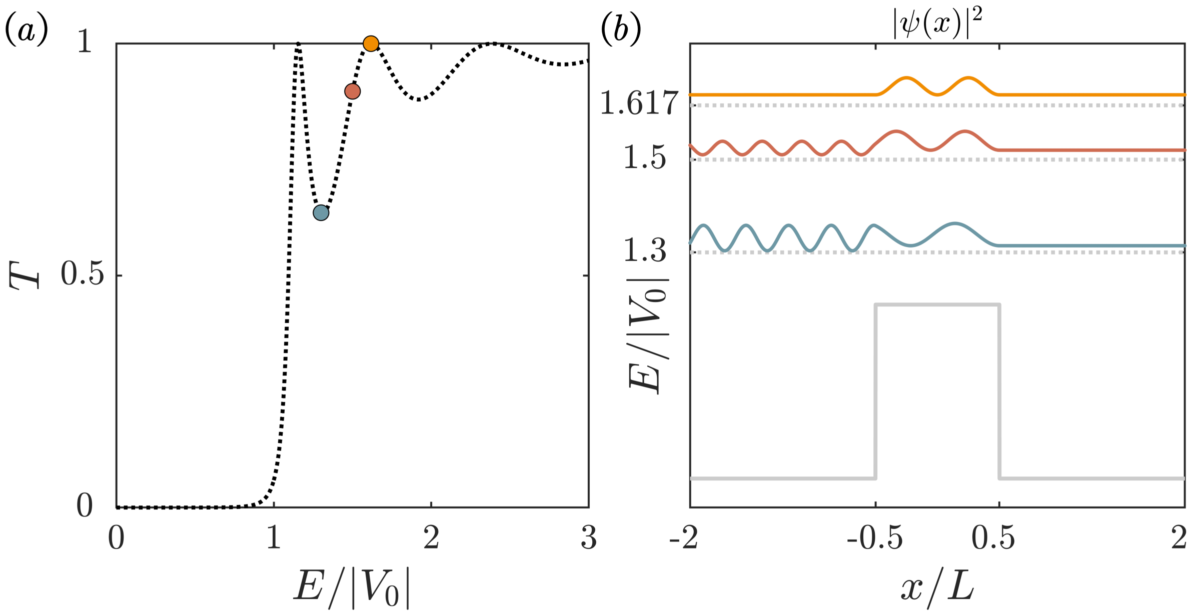

FIG. 7. (a) The transmission versus the energy of the particle $E/|V_0|$. (b) Probability distributions $|\psi_n(x)|^2$ as functions of x/L with different the energy of the particle. The dots in (a) are corresponding with the lines in (b) with same color. $V_0 = 32\hbar^2$J, the other parameters are the same as in Fig. (2).

(c)
Case I [Link]
Case II [Link]

Answer 2:

(a) double-slit experiment with single particles:

(b) Stern-Gerlach experiment:

(c) Aharonov-Bohm effect:
Electromagnetic potentials were initially introduced to obtain the canonical formalism and were long thought to have no independent significance, as in classical electrodynamics, the equations of motion can be fully expressed in terms of the electric and magnetic fields. In quantum mechanics, although the potentials cannot be eliminated from the fundamental equations, both the potentials and the equations are gauge invariant, so it seems that the potentials also have no independent significance in quantum mechanics.
However, in 1959, Aharonov and Bohm theoretically proposed that potentials can influence charged particles, even in regions where all fields (and thus the forces on the particles) vanish. This implies that potentials must, in certain cases, be considered physically significant, suggesting that potentials are fundamental physical entities, with fields derived from them through differentiation [*PR* **115**, 485 (1959)]. This phenomenon is now known as the Aharonov-Bohm effect and was experimentally observed in 1960 and 1986 [*PRL* **5**, 3 (1960)] [*PRL* **56**, 792 (1986)].
In the following sections, I will introduce the experimental achievements and derive the theory of the Aharonov-Bohm effect.

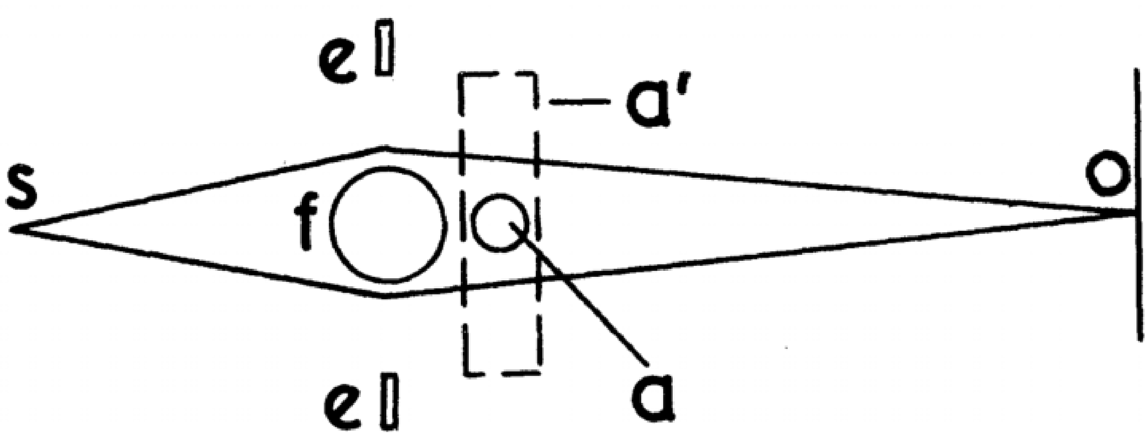

FIG. 8. The experimental system of Aharonov-Bohm effect. s is the source, e and f are the electrode of the biprism, which can deflexion the direction of the electrons. a and a′ are the confined and extended field regions, respectively. o is the observe plane.

Figure 8 shown the experimental system, s is the source, e and f are the electrode of the biprism, which can deflexion the direction of the electrons. a and a′ are the confined and extended field regions, respectively. o is the observe plane. In classical electrodynamics, the electron won't be affected when there exists a magnetic field, because there are no fields but only potentials in the path of the electron. However, in quantum mechanics, the probability wave have a phase difference, which causes interference.
The Hamiltonian of the electron with magnetic potential is

$$\hat{H} = \frac{1}{2m}(\hat{P} - e\vec{A})^2, \tag{32}$$

and the Schrödinger equation is

$$-\frac{1}{2m}(\nabla + \frac{ie}{\hbar})^2\psi(r,t) = E\psi(r,t). \tag{33}$$

We assume the solution $\psi(r,t) = \exp(-iEt/\hbar)\phi_0(r)\varphi(r)$, where $\phi_0(r)$ is the stationary state solution when there is no potential. Then we have the equation:

$$(\nabla + \frac{ie}{\hbar})\varphi(r) = 0, \tag{34}$$

therefore, the wavefunction is

$$\psi(r,t) = N\exp(-iEt/\hbar + i\int(\hat{P} - e\vec{A})/\hbar \cdot dl), \tag{35}$$

and there exit a phase difference when we calculate the probability along different path:

$$\begin{aligned}\Delta\phi &= -\frac{e}{\hbar}\int\int \nabla\times A\cdot dS + \frac{1}{\hbar}\oint p\cdot dl \\ &= -\frac{e}{\hbar}\Phi + \frac{1}{\hbar}\oint p\cdot dl,\end{aligned} \tag{36}$$

where Φ is magnetic flux.