Problem Set 2

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Problem 1. Let the initial wavefunction be defined by

$$\psi(x, t=0) = \frac{1}{\sqrt{2}}\left(\phi_1(x) - \phi_3(x)\right)$$

where $\phi_i(x)$ is the i^{th} lowest-energy eigenstate of the particle in a box.

(a) Give the analytic expression for the probability density.

(b) Give the analytic expression for the expected evolution of the probability density.

(c) Explain how the expected evolution of the probability density relates to the expected result for a nonstationary state.

(d) Give the analytic expression for the average position as a function of time.

Solution.

(a)

$$\begin{aligned}
\rho(x) &= |\Psi(x, t=0)|^2 \\
&= \frac{1}{2}\left(|\phi_1(x)|^2 + |\phi_3(x)|^2 - 2\mathrm{Re}\left(\phi_1^*(\mathrm{x})\,\phi_3(\mathrm{x})\right)\right) \\
&= \frac{1}{l}\left(\sin^2\left(\frac{\pi x}{l}\right) + \sin^2\left(\frac{3\pi x}{l}\right) - 2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)\right)
\end{aligned}$$

(b) Given the initial wavefunction, we have:

$$\Phi(x, t) = \frac{1}{2}\left(\phi_1(x)\,\mathrm{e}^{-iE_1 t/\hbar} - \phi_3(x)\,\mathrm{e}^{-iE_3 t/\hbar}\right)$$

then:

$$\begin{aligned}\rho(x,t) &= |\Psi(x,t)|^2 \\ &= \frac{1}{l}\left(\sin^2\left(\frac{\pi x}{l}\right)+\sin^2\left(\frac{3\pi x}{l}\right)-\mathrm{Re}\left(2\sin\left(\frac{\pi \mathrm{x}}{\mathrm{l}}\right)\sin\left(\frac{3\pi \mathrm{x}}{\mathrm{l}}\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\mathrm{E}_1-\mathrm{E}_3)\mathrm{t}}\right)\right) \\ &= \frac{1}{l}\left(\sin^2\left(\frac{\pi x}{l}\right)+\sin^2\left(\frac{3\pi x}{l}\right)-2\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)\cos\left(\frac{(E_1-E_3)}{\hbar}t\right)\right)\end{aligned}$$

where the evolution is:

$$\frac{\mathrm{d}\rho(x,t)}{\mathrm{d}t} = \frac{2}{l}\cdot\frac{E_1-E_3}{\hbar}\sin\left(\frac{\pi x}{l}\right)\sin\left(\frac{3\pi x}{l}\right)\sin\left(\frac{(E_1-E_3)}{\hbar}t\right)$$

(c) The system is in its nonstationary state, which means it can be expressed as superposition of stationary states. The expected evolution of the probability density is related to the interference of the stationary states, and is not 0.

(d)

$$\begin{aligned}\langle x\rangle &= \int_0^l \mathrm{d}x\ x\rho(x,t) \\ &= \frac{l}{2}\end{aligned}$$

which means superposition does not affect the average position.

Problem 2. Let the initial wavefunction be defined as the Gaussian wavepacket

$$\Psi(x,t=0) = N\mathrm{e}^{-a^2(x-L/2)^2/2}$$

where N is the normalization coefficient, $L = 5\text{Å}$, and $a = 4\text{Å}^{-1}$.

(a) Determine analytically whether $\Psi(x,t=0)$ is a stationary state for a particle-in-a-box potential.

(b) Using the accompanying Jupyter notebook:

i. Explain what the function $f(N) = \sum_{i=1}^{N} c_i^* c_i$ represents.

ii. Plot $f(N)$ for the given expansion coefficients c_i.

iii. Calculate $\lim_{N\to\infty} f(N)$.

iv. Explain what $f(N)$ says about the number of expansion terms required to accurately simulate the wavefunction..

v. Plot $|\Psi(x,t)|^2$ at several choices of t to show how the wavefunction changes in time.

vi. Explain what $|\Psi(x,t)|^2$ tells us about the motion os a particle in a box.

vii. Plot $\langle x(t)\rangle$ and $\left\langle (x-L/2)^2(t)\right\rangle$.

viii. Explain the significance of $\langle x(t)\rangle$ and $\left\langle (x-L/2)^2(t)\right\rangle$ and their relationships to $|\Psi(x,t)|^2$.

Solution.

(a) From normalization, we have:

$$N = \left(\frac{a^2}{\pi}\right)^{1/4}$$

For an in-box particle at $t=0$, the wavefunction could be expressed as:

$$\Psi(x, t=0) = \sum_i a_i \phi_i(x)$$

To determine whether $\Psi(x,t=0)$ is a stationary state, we need to check whether it is a superposition of eigenstates. Solve for c_i, we get:

$$\begin{aligned}
c_i &= \int_0^l \mathrm{d}x\ \Psi(x,t=0)\cdot\sqrt{\frac{2}{l}}\sin\left(\frac{i\pi x}{l}\right)\\
&= \int_{-\infty}^{\infty} \mathrm{d}x\ \Psi(x,t=0)\cdot\sqrt{\frac{2}{l}}\sin\left(\frac{i\pi x}{l}\right)\\
&= 2\frac{\pi^{1/4}}{\sqrt{la}}\sin\left(\frac{i\pi}{2}\right)\mathrm{e}^{-\frac{i^2\pi^2}{2a^2l^2}}
\end{aligned}$$

when i is odd, a_i is not zero, which means $\Psi(x,t=0)$ is not a stationary state.

(b) i. If we expand the wavefunction with particle-in-box eigenstates, it can be written as:

$$\Psi(x,t=0) = \sum_i c_i \phi_i(x)$$

For normalization, we have:

$$\sum_{i=1}^{\infty} |c_i|^2 = 1$$

which means $|c_i|^2$ is the probability of the particle in the i^{th} eigenstate. So $f(N) = \sum_i^N |c_i|^2$ is the probability of the particle in the first eigenstate to the N^{th} eigenstate.

ii. We can plot $f(N)$ as:

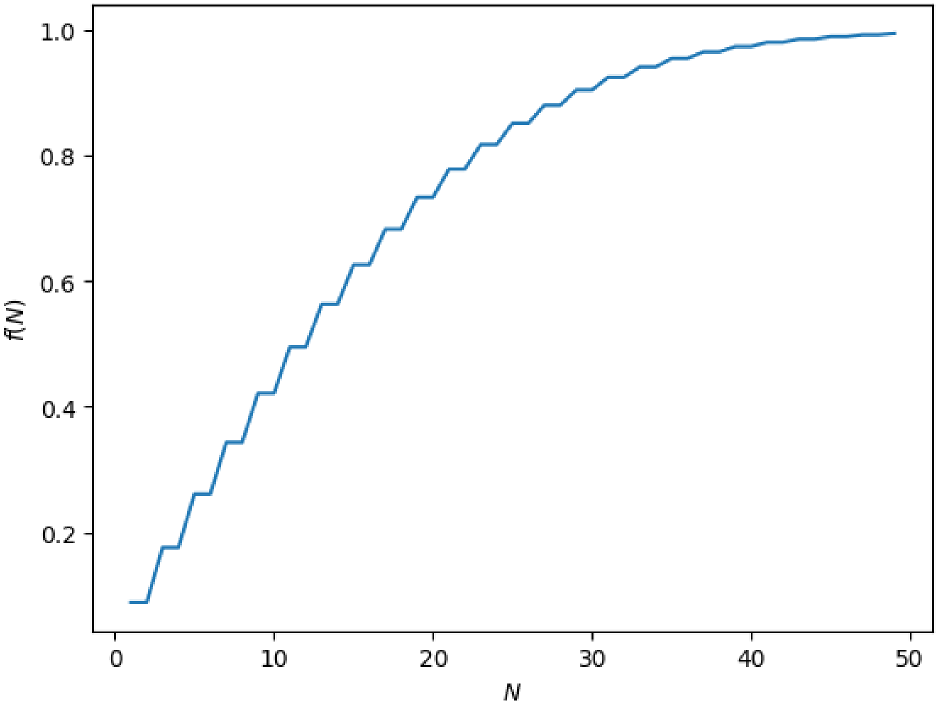

Figure 1: Plot of $f(N)$

iii. When $N \to \infty$, we can use intergral to calculate the limit:

$$\begin{aligned}\lim_{N\to\infty} f(N) &= \int_0^\infty \mathrm{d}i \ \ |c_i|^2 \\ &= \int_0^\infty \mathrm{d}i \ 4\left(\frac{\pi}{l^2a^2}\right)^{1/2} \sin^2\left(\frac{i\pi}{2}\right) \mathrm{e}^{-\frac{i^2\pi^2}{a^2l^2}} \\ &= 1 - \mathrm{e}^{-\frac{a^2l^2}{4}}\end{aligned}$$

assume that $al \gg 1$, we have:

$$\lim_{N\to\infty} f(N) \approx 1$$

iv. From the plot in Fig.1, we can see that when the number of extension terms is small, especially when $N < 20$, $f(N) < 0.8$, which means there's only 80% probability of the particle in the first 20 eigenstates. So to accurately simulate the wavefunction, we need to include more expansion terms. One great idea tis to connect the suitable number of expansion terms with la, which means to better fit the wavefunction, we should make $\frac{N}{al} \gg 1$.

v. Plots are as follows:

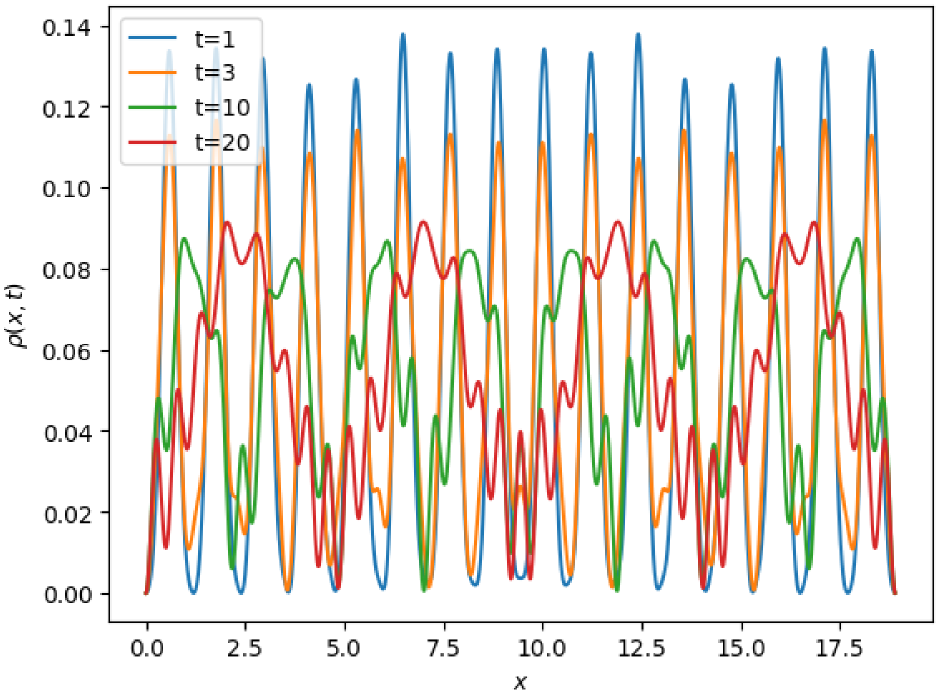

Figure 2: Plot of $|\Psi(x,t)|^2$

vi. Because the wavefunction is not a stationary state, the probability density will change in time. Due to the superposition, the density will form a peridic structure.

vii. Plots are as follows:

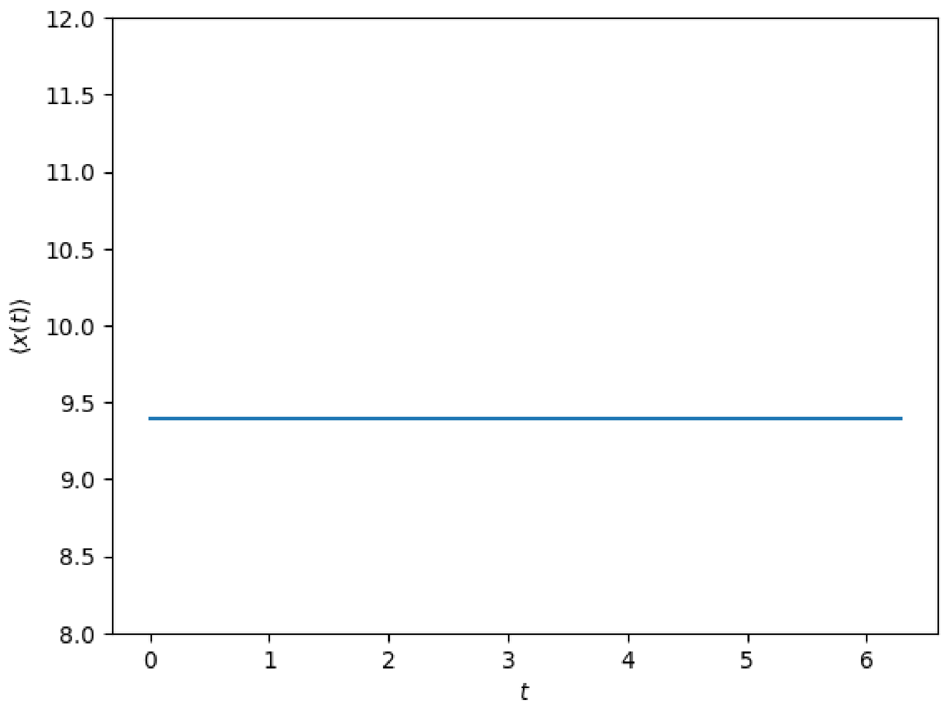

Figure 3: Plot of $\langle x\left(t\right)\rangle$

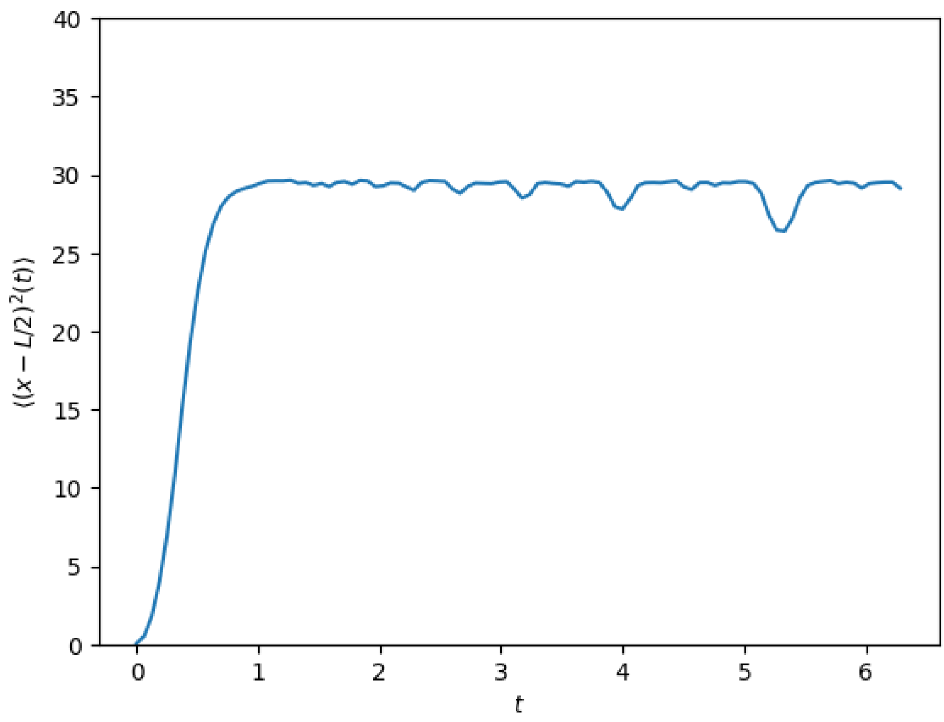

Figure 4: Plot of $\left\langle \left(x-L/2\right)^2\left(t\right)\right\rangle$

viii. From these plots, we can see that $\langle x\left(t\right)\rangle$ is constant with t, which means all of the eigenstates are centered at the same position, i.e., the middle of the box. And superposition does not affect the average position. $\left\langle (x - L/2)^2 (t) \right\rangle$ arises from 0 to a constant value, which means that superposition affects the density of the particle, but with enough time, the density will become uniform statistically, which makes $\left\langle (x - L/2)^2 (t) \right\rangle$ a constant and same value as when the density is uniform.