I. Time Evolution of a Wavepacket

A particle is initially in the ground state of a harmonic oscillator potential. It then evolves freely in time (the potential is turned off).

(a) Use the free-particle propagator to determine the time evolution of its wavefunction.

Solution:
A wave function propagating through space and time is expressed as

$$\psi(\mathbf{x}'', t) = \int \mathrm{d}^3x' K(\mathbf{x}'', t; \mathbf{x}', t_0)\psi(\mathbf{x}', t_0) \tag{1}$$

where $K(x'', t; x', t_0)$ is the propagator and $\psi(x', t_0)$ is the initial wave function. Given that the particle is initially in the ground state of a harmonic oscillator potential, $\psi(x', t_0)$ is

$$\psi(x', t_0) = \frac{1}{\pi^{1/4}\sqrt{x_0}} \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \tag{2}$$

where $x_0 = \sqrt{\hbar/(m\omega)}$. On the other hand, the free-particle propagator is

$$K(x'', t; x', t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left[\frac{im\,(x''-x')^2}{2\hbar(t-t_0)}\right] \tag{3}$$

Substituting Eqs. (2) and (3) into a one-dimensional form of Eq. (1) and integrating over all space, we have

$$\begin{aligned}
\psi(x'', t) &= \int_{-\infty}^{\infty} \mathrm{d}x' \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left[\frac{im\,(x''-x')^2}{2\hbar(t-t_0)}\right] \cdot \frac{1}{\pi^{1/4}\sqrt{x_0}} \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \\
&= \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \sqrt[4]{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[\frac{im\,(x''-x')^2}{2\hbar(t-t_0)}\right] \exp\left[-\frac{m\omega x'^2}{2\hbar}\right] \\
&= \omega^{1/4}\sqrt{\left(\frac{m}{\pi\hbar}\right)^{3/2} \frac{1}{2i(t-t_0)}} \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[\frac{imx''^2 + imx'^2 - 2imx''x' - m\omega(t-t_0)x'^2}{2\hbar(t-t_0)}\right] \\
&= A(t) \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[\frac{(im - m\omega(t-t_0))x'^2 - 2imx''x' + imx''^2}{2\hbar(t-t_0)}\right] \\
&= A(t) \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[-\frac{m(\omega(t-t_0)-i)}{2\hbar(t-t_0)}\left(x'^2 + \frac{2ix''}{\omega(t-t_0)-i}x' - \frac{ix''^2}{\omega(t-t_0)-i}\right)\right] \\
\psi(x'', t) &= A(t) \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[-B(t)\left(x'^2 + 2\alpha(x'', t)x' - \beta(x'', t)\right)\right]
\end{aligned} \tag{4}$$

by replacing some terms as

$$\begin{aligned}
A(t) = \omega^{1/4}\sqrt{\left(\frac{m}{\pi\hbar}\right)^{3/2} \frac{1}{2i(t-t_0)}}, &\quad B(t) = -\frac{m(\omega(t-t_0)-i)}{2\hbar(t-t_0)}, \\
\alpha(x'', t) = \frac{ix''}{\omega(t-t_0)-i}, &\quad \beta(x'', t) = \frac{ix''^2}{\omega(t-t_0)-i}
\end{aligned} \tag{5}$$

We can complete the square where $(b/(2a))^2 = ((2\alpha)/2)^2 = \alpha^2$ on the quadratic equation to obtain

$$x'^2 + 2\alpha x' - \beta + \alpha^2 - \alpha^2 = (x+\alpha)^2 - \beta - \alpha^2 = (x+\alpha)^2 + C \tag{6}$$

Using this, we can rearrange Eq. (4) as

$$\begin{aligned}\psi(x'',t) &= A(t)\int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[-B(t)\left(\left(x'^2+\alpha(x'',t)\right)^2 + C(x'',t)\right)\right] \\ &= A(t)\,\exp\left[-B(t)C(x'',t)\right]\int_{-\infty}^{\infty}\mathrm{d}x' \exp\left[-B(t)\left(x'+\alpha(x'',t)\right)^2\right]\end{aligned} \tag{7}$$

Let $u = x' + \alpha$ which leads to $\mathrm{d}u = \mathrm{d}x'$. Changing variables, we have

$$\psi(x'',t) = A(t)\,\exp\left[-B(t)C(x'',t)\right]\int_{-\infty}^{\infty}\mathrm{d}u \exp\left[-B(t)u^2\right] \tag{8}$$

Note that the Gaussian integral is

$$\int_{-\infty}^{\infty} e^{-ax^2}\mathrm{d}x = \sqrt{\frac{\pi}{a}} \tag{9}$$

Applying this, Eq. (8) becomes

$$\psi(x'',t) = A(t)e^{-B(t)C(x'',t)}\sqrt{\frac{\pi}{B(t)}} \tag{10}$$

which gives the time evolution of the wavefunction in this scenario.

(b) Determine how the probability density spreads in time.

Solution:
To better see the form of the probability density, we express $C(x'',t)$ as

$$\begin{aligned}C(x'',t) &= -\beta(x'',t) - \alpha(x'',t)^2 \\ &= -\frac{ix''^2}{\omega(t-t_0)-i} - \left(\frac{ix''}{\omega(t-t_0)-i}\right)^2 \\ &= \left[\frac{1}{(\omega(t-t_0)-i)^2} - \frac{i}{\omega(t-t_0)-i}\right]x''^2 \\ C(x'',t) &= \gamma(t)x''^2\end{aligned} \tag{11}$$

Then, the probability density is calculated to be

$$\rho(x'',t) = |\psi(x'',t)|^2 = \frac{\pi A(t)^2}{B(t)}e^{-2B(t)C(x'',t)} = \frac{\pi A(t)^2}{B(t)}e^{-2B(t)\gamma(t)x''^2} \tag{12}$$

where we see $\rho(x'',t)$ as some kind of Gaussian distribution.

References

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Sakurai, *Modern Quantum Mechanics*, Chapter 2, Section 5

II. Aharanov-Bohm Effect

Describe how the Aharanov-Bohm effect can be used to measure magnetic flux through a tight solenoid by an interferometer experiment.

Answer:
Let the tight solenoid be very long and impenetrable so that there is no magnetic field that can be detected outside of it. However, inside it is a uniform magnetic field **B** that runs parallel along the length of the solenoid. As we send a beam of electrons towards the solenoid and split it so that some electrons take either the path above or below the solenoid, we observe an interference pattern in the region past the solenoid. The presence of **B** inside the solenoid affects the phase difference of the two split beams, and in effect, the observed interference pattern due to the non-zero vector potential outside. Since the phase difference between the two paths is proportional to the magnetic flux inside the solenoid, we can calculate for the phase difference to obtain the magnetic flux.

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III. Density Operator

(a) Explain why all wavefunctions describe pure states.

Answer:
Pure states are quantum states that cannot no longer be decomposed into more fundamental states. Any other state that is not a pure state (mixed state) can generally be written as a linear combination of pure states. Wavefunctions, on the other hand, are the mathematical depictions of quantum states for a certain system. Therefore, all wavefunctions describe pure states as all states can be expressed by such states.

(b) Write down the matrix elements of a density operator ρ in the eigenbasis $|n\rangle$. Explain why the eigenvalue spectrum of a density operator always corresponds to a probability distribution.

Solution:
The density operator is defined to be

$$\rho \equiv \sum_{k}^{N} p_k \left|\psi_k\right\rangle \left\langle\psi_k\right| \tag{13}$$

where $\{|\psi_k\rangle\}$ is a set of pure states, p_k are weights that satisfy $0 < p_k \leq 1$ and the normalization condition

$$\sum_{k}^{N} p_k = 1 \tag{14}$$

Note that this form of ρ is for a mixed state but it can be specified to pure states.

An example of a situation involving mixed states is when we consider a system consisting of N particles. The state of a particle, which will be described in the eigenbasis $|n\rangle$ and may have a different probability in occupying $|n\rangle$ with another particle, is expressed as

$$|\psi_k\rangle = \sum_n c_n^k |n\rangle \tag{15}$$

where $k = 1, \ldots, N$ and c_n^i are complex coefficients. Then, the density operator in Eq. (13) takes the form of

$$\begin{aligned}\rho &= \sum_k^N \sum_{n,m} p_k \left(c_n^k |n\rangle\right) \left(\left(c_m^k\right)^* \langle m|\right) \\ &= \sum_k^N \sum_{n,m} p_k c_n^k \left(c_m^k\right)^* |n\rangle \langle m|\end{aligned} \tag{16}$$

which has matrix components expressed as

$$\begin{aligned}\langle m|\rho|n\rangle &= \sum_k^N p_k c_n^k \left(c_m^k\right)^* \langle m|n\rangle \langle m|n\rangle \\ &= \sum_k^N p_k c_n^k \left(c_m^k\right)^* (\langle m|n\rangle)^2\end{aligned} \tag{17}$$

For diagonal terms $(n = m)$, we get

$$\langle n|\rho|n\rangle = \sum_k^N p_k c_n^k \left(c_n^k\right)^* \left(\cancelto{1}{\langle n|n\rangle}\right)^2 = \sum_k^N p_k |c_n^k|^2 \tag{18}$$

where $|c_n^k|^2$ is the probability that a system depicted by ψ_k will be observed in the basis state $|n\rangle$. Therefore, the diagonal terms given by $\langle n|\rho|n\rangle$ gives the probability that the whole system will be observed in $|n\rangle$. This shows that the eigenvalue spectrum of ρ corresponds to a probability distribution.

References

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