Quantum Mechanics I

Week Easter (Solutions)

Spring Semester 2025

1 Particle in an uniform electric field

An electron is known to be initially in a state with zero average momentum $\bar{p}(0) = \langle p \rangle = 0$, and is known to be described at $t = 0$ by a real-valued wavefunction. The electron can be assumed to move in one dimension (along the x axis). An uniform and time-independent electric field E parallel to the x axis is turned on to accelerate the electron.

(a) Write the Hamiltonian of the system and the corresponding time-dependent Schrödinger equation.

The Hamiltonian can be written as the sum of the kinetic energy $\hat{p}^2/(2m_e)$ and of the electrostatic potential of the electron in the external field: $\hat{V} = eE\hat{x}$, where $\hat{x}$ is the position operator. Thus

$$\hat{H} = \frac{\hat{p}^2}{2m_e} + eE\hat{x} \ . \tag{1.1}$$

The time-dependent Schrödinger equation then reads:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + eEx\psi \tag{1.2}$$

and, taking into account that the particle is assumed to move only in one dimension,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2\partial^2\psi(x,t)}{\partial x^2} + eEx\psi(x,t) \ . \tag{1.3}$$

(b) Write and solve the corresponding Heisenberg equations of motion and compute the average position and momentum at time t.

The Heisenberg equations of motion read:

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H},\hat{x}] = \frac{i}{2m\hbar}(\hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p}) = \frac{\hat{p}}{m} \ , \tag{1.4}$$

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H},\hat{p}] = \frac{i}{\hbar}eE[\hat{x},\hat{p}] = -eE \ . \tag{1.5}$$

The solutions of the Heisenberg equations can be derived by integrating the equations of motion and give:

$$\begin{aligned}\hat{p}(t) &= -eEt\hat{1} + \hat{p}(0) \ , \\ \hat{x}(t) &= \hat{x}(0) - \frac{eEt^2}{2m}\hat{1} + \frac{\hat{p}(0)t}{m}\end{aligned} \tag{1.6}$$

Here, $\hat{1}$ is used to denote the identity operator (an operator which acts trivially on every state vector in the Hilbert space, i.e. $\hat{1}|\psi\rangle = |\psi\rangle$. The $\hat{1}$ operator commutes with all operators: $[\hat{1}, \hat{A}] = 0$ for any $\hat{A}$.

The average position and momentum at time t can be expressed as

$$\begin{aligned} \bar{x}(t) &= \langle\psi_0|\hat{x}(t)|\psi_0\rangle = \bar{x}(0) - \frac{eEt^2}{2m} + \frac{\bar{p}(0)t}{m} \\ \bar{p}(t) &= \langle\psi_0|\hat{p}(t)|\psi_0\rangle = \bar{p}(0) - eEt \ , \end{aligned} \tag{1.7}$$

where $|\psi_0\rangle$ is the state vector in the Heisenberg picture. We can see that the average position and momentum describe the same trajectory of a corresponding classical particle. Assuming that $\bar{p}(0) = 0$, we can further simplify the expressions, obtaining:

$$\begin{aligned} \bar{x}(t) &= \bar{x}(0) - \frac{eEt^2}{2m} \\ \bar{p}(t) &= -eEt \ , \end{aligned} \tag{1.8}$$

(c) Calculate the uncertainties in the position and the momentum of the particle at time t.

Hint. The calculation should show that $(\Delta x(t))^2$ contains a term proportional to the average $\langle\psi_0|\hat{x}(0)\hat{p}(0) + \hat{p}(0)\hat{x}(0)|\psi_0\rangle$. This average can be shown to be equal to zero if it is assumed that the wavefunction at $t = 0$ is real-valued. Can you show this?

To determine the uncertainties we can compute

$$\begin{aligned} \langle(x(t) - \bar{x}(t))^2\rangle &= \langle\psi_0| \left(\hat{x}(t) - \bar{x}(0) + \frac{eEt^2}{2m}\hat{1} - \frac{\bar{p}(0)}{m}t\right)^2 |\psi_0\rangle \\ &= \langle\psi_0| \left(\hat{x}(0) - \bar{x}(0) + \frac{(\hat{p}(0) - \bar{p}(0))t}{m}\right)^2 |\psi_0\rangle \\ &= (\Delta x(0))^2 + \frac{t^2}{m^2}(\Delta p(0))^2 \\ &+ \frac{t}{m}\langle\psi_0|(\hat{x}(0)\hat{p}(0) + \hat{p}(0)\hat{x}(0))|\psi_0\rangle \ . \end{aligned} \tag{1.9}$$

$$\langle(p(t) - \bar{p}(t))^2\rangle = \langle\psi_0| \left(\hat{p}(0) - \bar{p}(0)\right)^2 |\psi_0\rangle = (\Delta p(0))^2 \ . \tag{1.10}$$

We see that the time-dependence of the uncertainties does not depend on the external electric field. Thus, the uncertainties evolve in the same way as they would for a free particle in absence of an external potential. The results show that the uncertainty in the momentum is constant in time. This is expected because the electron is subject to a force which is constant, so its momentum is simply shifted in time by a term $-eEt$. If we were to know the momentum exactly at time $t = 0$, then we would know it exactly also at any later time: simply it would be the initial momentum $-eEt$.

The uncertainty in the position has three terms. The first is the initial uncertainty $\Delta x(0)$. The second, $(\Delta p(0))^2 t^2/m^2$ has a simple classical interpretation: the uncertainty in the initial velocity leads to an additional error in our prediction of the position at later times. This error adds (in quadrature) to the error $(\Delta x(0))^2$.

The last term, proportional to $\langle\psi_0|(\hat{x}(0)\hat{p}(0) + \hat{p}(0)\hat{x}(0))|\psi_0\rangle$ can be simplified in the following way. The Heisenberg-picture state $|\psi_0\rangle$ coincides with the Schrödinger picture state at $t = 0$, and is assumed to be real-valued.

Then:

$$\begin{aligned}\langle\psi_0|(\hat{x}(0)\hat{p}(0) + \hat{p}(0)\hat{x}(0))|\psi_0\rangle &= -i\hbar \int_{-\infty}^{\infty} dx \psi_0^*(x) \left(x\frac{d}{dx}\psi_0(x) + \frac{d}{dx}(x\psi_0(x)\right) \\ &= -i\hbar \int_{-\infty}^{\infty} dx \frac{d}{dx}\left(x\psi_0^2\right) = 0\end{aligned} \tag{1.11}$$

for $\psi_0(x)$ real-valued. So we get simply that $\Delta x^2(t) = \Delta x^2(0) + \Delta p^2 t^2/m^2$.

In general, however, the cross term does not vanish.

2 Diffraction and the uncertainty principle

A beam of electrons, traveling in the $+z$ direction, is sent against a screen with a circular aperture of radius R. The electrons in the beam have initial momentum $\mathbf{p} = \hbar(0, 0, k)$, $k > 0$, and the screen with the aperture is located in the plane $z = 0$. In a plane $z = L$ a second screen, parallel to the first, is used to detect the intensity of the diffracted beam.

(a) Using the uncertainty principle, estimate the characteristic size of the diffraction pattern (in other words, the size of the region on the detector screen at which the intensity is not negligible). Assume that $kR \gg 1$.

After the electon has passed through the aperture in the first screen, we acquire knowledge on its x, y coordinates, which were undetermined initially. The coordinates of the electrons, in particular, become known with an accuracy of order $\Delta x \simeq R$, $\Delta y \simeq R$. By the uncertainty principle, this means that the transverse components of the momenta must become uncertain, with uncertainties $\Delta p_x \geq \hbar/(2\Delta x) \simeq \hbar/(2R)$ and $\Delta p_y \geq \hbar/(2\Delta y) = \hbar/(2R)$. If $kR \gg 1$, these uncertainties are much smaller than the initial value of the momentum. Thus the electron move almost in straight motion.

The small angle between the direction of propagation (p_x, p_y, p_z) and the z axis can be calculated as:

$$\cos\theta = \frac{p_z}{|\mathbf{p}|} . \tag{2.1}$$

The modulus $|\mathbf{p}|$ after the screen is equal to the modulus of the initial momentum p by energy conservation. This can be seen in two ways. One way is to note that the problem may be described using a Hamiltonian in which the screen is described as a potential barrier, stopping the electrons away from the aperture. Since the Hamiltonian is time-independent, the energy must be conserved.

A second way, more precise, is to note that the screen has a very large mass compared to that of the electron. Due to the large differences in the mass $M_{\text{screen}} \gg m_e$, the energy absorbed by the screen as it recoils due to the collision with the electron is completely negligible.

For $kR \gg 1$, we can approximate Eq. (2.1) by keeping only the leading term in the Taylor expansion near $\theta = 0$

$$1 - \frac{\theta^2}{2} \simeq \frac{1}{\sqrt{\pi R^2}} \sqrt{1 - \frac{p_x^2 + p_y^2}{p^2}} = 1 - \frac{p_x^2 + p_y^2}{2p^2} \ . \tag{2.2}$$

So we obtain that the variance of the angle is

$$\Delta\theta^2 = \frac{1}{p^2} \left(\Delta p_x^2 + \Delta p_y^2\right) \simeq \frac{\hbar^2}{2R^2 p^2} = \frac{1}{2k^2 R^2} \ , \tag{2.3}$$

and its standard deviation $\Delta\theta \simeq 1/(\sqrt{2}kR)$. The intensity distribution on the detector screen must, therefore, be a spot of size $r_L \simeq L\Delta\theta \simeq L/(\sqrt{2}kR)$. (The factor need not need accurate, but for sure the size of the spot is proportional to $L/(kR)$.)

(b) Describe qualitatively what happens if, instead, $kR \ll 1$.

In the opposite limit $kR \ll 1$, the uncertainty in the momentum becomes large and the electrons do not travel in an almost straight line. Rather, the electrons emerging after the aperture form approximately a spherical wave.

(c) Quantum mechanically, an approximate solution for the diffracted beam in the region far from the aperture and for small angles is given by[1]:

$$\psi(\mathbf{r}) = -\frac{1}{2\pi} \int_{x',y'} \psi(x', y') \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \ . \tag{2.4}$$

Here x', y' run over all points on the plane $z = 0$ and $\mathbf{r}' = (x', y', 0)$. This formula expresses mathematically the Huygens principle: the wavefunction at all points in space can be calculated by considering a single wavefront and by considering every point on the wavefront as a source of spherical waves. In the case of interest here, we can take $\psi(x', y') = \psi_0$ if $x'^2 + y'^2 < R^2$, $\psi(x', y') = 0$ otherwise with ψ_0 a constant. Using Eq. (2.4) and approximating for $L \gg R$, show that the intensity distribution on the screen can be expressed in terms of the Fourier transform

$$\int_{x',y'} \psi(x', y') e^{-iq_x x' - iq_y y'} = \psi_0 \int_0^{2\pi} d\theta' \int_0^R r' \ dr' e^{-iq_x x' - iq_y y'} \ , \tag{2.5}$$

where $x' = r' \cos\theta'$, $y' = t' \sin\theta'$.

For $L \gg R$, that is, when the detector screen is located at large distance compared to the size of the aperture, we can approximate Eq. (2.4) replacing $1/|\mathbf{r} - \mathbf{r}'| \simeq 1/|\mathbf{r}|$. In the exponential factor $e^{ik|\mathbf{r}-\mathbf{r}'|}$, we can approximate

$$|\mathbf{r} - \mathbf{r}'| \simeq |\mathbf{r}| - \frac{\mathbf{r} \cdot \mathbf{r}'}{|\mathbf{r}|} \ , \qquad \mathbf{r} = (x, y, z) \ . \tag{2.6}$$

[1] A more accurate solution can be constructed using the Rayleigh-Sommerfeld diffraction theory.

Since $\mathbf{r}' = (x', y', 0)$ has no z component, $\mathbf{r}\cdot\mathbf{r}' = xx' + yy'$ and defining $q_x = -kx/|\mathbf{r}|$, $q_y = -ky/|\mathbf{r}|$, we can rewrite:

$$\psi(\mathbf{r}) = -\frac{e^{ik|\mathbf{r}|}}{2\pi|\mathbf{r}|}\int_{x',y'} \psi(x', y')e^{-ik(xx'+yy')/|\mathbf{r}|} \tag{2.7}$$

Introducing $q_x = kx/|\mathbf{r}|$, $q_y = ky/|\mathbf{r}|$ we can write the intensity as

$$I(\mathbf{r}) \propto |\psi(\mathbf{r})|^2 \propto \frac{1}{4\pi^2|\mathbf{r}|^2}\left|\int_{x',y'} \psi(x', y')e^{-i(q_x x'+q_y y')}\right|^2 . \tag{2.8}$$

We see that there is a relation between the intensity and the Fourier transform of the wavefunction on the plane $z = 0$.

(d) To simplify the calculation, approximate the amplitude after the aperture with a Gaussian wavefunction of spread R:

$$\psi(x', y') = \frac{\psi_0}{\sqrt{2}}e^{-(x'^2+y'^2)/(4R^2)} . \tag{2.9}$$

With this simplification and assuming a small scattering angle (so that $|\mathbf{r}| \simeq L$) calculate analytically the intensity distribution on the screen.

Show that the width of the distribution matches with the one estimated using the uncertainty principle.

By explicit calculation we find

$$\begin{aligned} I(x', y') &\propto \frac{|\psi_0|^2}{8\pi^2|\mathbf{r}|^2}\left|\int_{x',y'} dx'dy' e^{-(x'^2+y'^2)/(4R^2)-iq_x x'-iq_y y'}\right|^2 \\ &= \frac{|\psi_0|^2}{\pi^2|\mathbf{r}|^2}(4\pi R^2)^2 e^{-2(q_x^2+q_y^2)R^2} = 16|\psi_0|^2\frac{R^2}{|\mathbf{r}|^2}e^{-2(q_x^2+q_y^2)R^2} . \end{aligned} \tag{2.10}$$

Recalling that $q_x = kx/|\mathbf{r}|$, $q_y = ky/|\mathbf{r}|$ and considering small scattering angles so that $|\mathbf{r}| \simeq L$ we get

$$I(x', y') \simeq 16|\psi_0|^2\frac{R^2}{L^2}e^{-2(x^2+y^2)k^2R^2/L^2} . \tag{2.11}$$

The intensity of the screen has a gaussian shape, and has width $\Delta x = \Delta y = L/(2kR)$. Up to a factor we recover the result estimated from the uncertainty principle.

3 Coherent States

In this exercise, we consider further properties and consequences of the harmonic oscillator, and more importantly we will introduce a class of states that are of great significance in condensed matter physics and quantum optics, the coherent states.

(a) For the stationary states of the harmonic oscillator $|n\rangle$, show that:

$$\sigma_x \, \sigma_p = \frac{\hbar}{2}(2n+1), \tag{3.1}$$

and thus only the ground state of the harmonic oscillator attains the uncertainty limit.

The dispersions in position and momentum are given by

$$\sigma_x^2 = \langle n|x^2|n\rangle - \langle n|x|n\rangle^2 , \quad \sigma_p^2 = \langle n|p^2|n\rangle - \langle n|p|n\rangle^2 .$$

We have shown already that the expectation values of position and momentum with respect to the harmonic oscillator stationary states are zero, i.e. $\langle n|x|n\rangle = \langle n|p|n\rangle = 0$. The rest of the expectation values we obtain them by using the results of Exercise 1 of Week 8 (Harmonic Oscillator):

$$\langle n|x^2|n\rangle = \frac{\hbar}{2m\omega}(2n+1), \quad \langle n|p^2|n\rangle = \frac{\hbar m\omega}{2}(2n+1).$$

Taking the product of the dispersions, we find

$$\sigma_x\sigma_p = \left[\sqrt{\frac{\hbar}{2m\omega}}\sqrt{2n+1}\right] \cdot \left[\sqrt{\frac{\hbar m\omega}{2}}\sqrt{2n+1}\right] = \frac{\hbar}{2}(2n+1).$$

The ground state $n=0$ minimizes the uncertainty product, since $\sigma_x\sigma_p = \frac{\hbar}{2}$.

(b) Certain linear combinations (known as coherent states) also minimize the uncertainty product. They are in fact eigenstates of the lowering operator:

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \,, \tag{3.2}$$

where α is complex. Show that indeed these states achieve the uncertainty limit.

We first consider the dispersion in the position with respect to the coherent state:

$$\sigma_x^2 = \langle\alpha|x^2|\alpha\rangle - \langle\alpha|x|\alpha\rangle^2 .$$

Using the expression for the position operator in terms of the ladder operators, $\hat{x} = x_0(\hat{a}+\hat{a}^\dagger)$, $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$ we find:

$$\langle\alpha|x|\alpha\rangle = x_0\,\langle\alpha|(a+a^\dagger)|\alpha\rangle = x_0(\alpha+\alpha^*) = 2x_0 Re\{\alpha\},$$

and for the second moment,

$$\begin{aligned}\langle\alpha|x^2|\alpha\rangle &= x_0^2\,\langle\alpha|(a+a^\dagger)^2|\alpha\rangle \\ &= x_0^2[\alpha^2 + (\alpha^*)^2 + 1 + 2\alpha^*\alpha] \\ &= x_0^2[4Re\{\alpha\}^2 + 1].\end{aligned}$$

In the second line, we used $aa^\dagger = 1 + a^\dagger a$, a consequence of the commutator $[a, a^\dagger] = 1$. Then, using the latter two results, we find:

$$\sigma_x^2 = x_0^2[4Re\{\alpha\}^2+1] - 4x_0^2 Re\{\alpha\}^2 = x_0^2,$$

and thus $\sigma_x = x_0$.

In a very similar fashion, we now proceed with the uncertainty in the momentum operator with respect to the coherent state,

$$\sigma_p^2 = \langle\alpha|p^2|\alpha\rangle - \langle\alpha|p|\alpha\rangle^2 .$$

Using the expression of the momentum operator in terms of the ladder operators, i.e. $p = ip_0(a^\dagger - a)$, $p_0 = \sqrt{\frac{\hbar m\omega}{2}}$, we have:

$$\langle\alpha|p|\alpha\rangle = ip_0 \langle\alpha|(a^\dagger - a)|\alpha\rangle = ip_0(\alpha^* - \alpha) = p_0 2Im\{\alpha\}$$

and for the second moment

$$\begin{aligned}\langle\alpha|p^2|\alpha\rangle &= -p_0^2 \langle\alpha|(a^\dagger - a)^2|\alpha\rangle \\ &= -p_0^2\Big[-4Im\{\alpha\}^2 - 1\Big] \\ &= p_0^2\Big[4Im\{\alpha\}^2 + 1\Big]\end{aligned}$$

The uncertainty in the momentum can be calculated:

$$\sigma_p^2 = p_0^2\Big[4Im\{\alpha\}^2 + 1\Big] - 4p_0^2 Im\{\alpha\}^2 = p_0^2,$$

and thus $\sigma_p = p_0$. Then, the uncertainty product becomes :

$$\sigma_x\sigma_p = x_0 p_0 = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}} = \frac{\hbar}{2} \tag{3.3}$$

and thus indeed the coherent state also minimizes the uncertainty product.

(c) Like any other state, a coherent state can be expanded in terms of the energy eigenstates:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle .. \tag{3.4}$$

Show that the expansion coefficients are

$$c_n = \frac{\alpha^n}{\sqrt{n!}} c_0. \tag{3.5}$$

The expansion coefficients corresponds to overlaps of the energy eigenstates with the coherent state, i.e. $c_n = \langle n|\alpha\rangle$. The n-th eigenstate is obtained by applying the raising operator n times (with suitable coefficient), i.e.

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle .$$

Using this fact, the coefficients are

$$c_n = \langle n|\alpha\rangle = \langle 0| \frac{(a)^n}{\sqrt{n!}} |\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}} c_0.$$

(d) Determine c_0 by normalizing $|\alpha\rangle$.

$$\begin{aligned}\langle\alpha|\alpha\rangle &= \Big(\sum_n c_n^* \langle n|\Big)\Big(\sum_n c_m |m\rangle\Big) = \\ &= \sum_{n,m} c_n^* c_m \langle n|m\rangle = \\ &= \sum_{n,m} c_n^* c_m \delta_{n,m} = \\ &= \sum_n |c_n|^2\end{aligned}$$

Then, using the result of the previous question, we write:

$$\begin{aligned}\langle\alpha|\alpha\rangle &= \sum_n |c_n|^2 = \\ &= \sum_n \frac{(|\alpha|^2)^n}{n!}|c_0|^2 = \\ &= e^{|\alpha|^2}|c_0|^2.\end{aligned}$$

Since we require normalization of the coherent state, i.e. $\langle\alpha|\alpha\rangle = 1$, we find:

$$c_0 = e^{-|\alpha|^2/2}.$$

The coefficients take the following form

$$c_n = \frac{\alpha^n}{\sqrt{n!}}e^{-|\alpha|^2/2},$$

and the resulting distribution is

$$P(n;\mu = |\alpha|^2) = |c_n|^2 = e^{-|\alpha|^2}\frac{(|\alpha|^2)^n}{n!}.$$

The distribution formed by $|c_n|^2$ with respect to n is a Poisson distribution form, where $|\alpha|^2$ correspond to the mean of the distribution.

(e) Show that a coherent state can be expressed as

$$|\alpha\rangle = D(\alpha)\,|0\rangle\,, \quad \text{where} \quad \hat{D}(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}, \tag{3.6}$$

where $D(\alpha)$ is called the 'displacement' operator, for reasons that will be obvious later on, and it is a unitary operator.

Hint: The Baker–Campbell–Hausdorff formula will be useful

$$e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]},$$

where the two operators X, Y have the following commutation relations: $[X, Y] = c$ and $[X, [X, Y]] = [Y, [Y, X]] = 0$.

We have shown that

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} c_0 |n\rangle$$

which can be expressed in terms of the ground state $|0\rangle$ using $|n\rangle = (a^\dagger)^n / \sqrt{n!}\, |0\rangle$,

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle = c_0 \sum_{n=0}^{\infty} \frac{(\alpha a^\dagger)^n}{n!} |0\rangle .$$

We use the expression for $c_0 = \exp\{-|\alpha|^2/2\}$ from the previous question to write

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha a^\dagger)^n}{n!} |0\rangle .$$

From the Taylor expansion of the exponential, we find:

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle .$$

To proceed, we consider the Baker–Campbell–Hausdorff formula for $\hat{X} = \alpha \hat{a}^\dagger$ and $\hat{Y} = -\alpha^* \hat{a}$.

$$e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]},$$

where the "higher-order" commutators are zero. The commutator evaluates to $|\alpha|^2$ and thus:

$$e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} e^{-|\alpha|^2/2} = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}}. \tag{3.7}$$

At a first glance, this result does not seem to be useful in our expression, but a closer look does the trick. Consider the action of the LHS on $|0\rangle$,

$$e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} e^{-|\alpha|^2/2} |0\rangle = e^{-|\alpha|^2/2} \sum_{n,m} \frac{\alpha^n (\alpha^*)^m}{n! m!} (\hat{a}^\dagger)^n \hat{a}^m |0\rangle .$$

The action of the lowering operator on the ground state gives zero, thus the only terms remaining are the ones for $m = 0$, which corresponds to the following results

$$e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} e^{-|\alpha|^2/2} |0\rangle = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |0\rangle .$$

The latter is equal to $|\alpha\rangle$. At the same time, using the result of Eq. (3.7), we find:

$$|\alpha\rangle = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} |0\rangle . \tag{3.8}$$

We thus identify

$$\hat{D}(\alpha) = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} \tag{3.9}$$

as the displacement operator, and it's indeed a unitary operator.

(f) To gain some insights on our earliest result, first find an expression for the real and imaginary parts of α in terms of the expectation values of the position and momentum operators (in the coherent state). Hint: Consider the expectation values first.

First, the position operator written in terms of the ladder operators,

$$\hat{x} = \frac{\ell_0}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right), \quad \ell_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

The expectation value is taken with respect to the coherent state as follows:

$$\langle\alpha|\hat{x}|\alpha\rangle = \frac{\ell_0}{\sqrt{2}}\langle\alpha|\left(\hat{a} + \hat{a}^\dagger\right)|\alpha\rangle = \frac{\ell_0}{\sqrt{2}}\left(\alpha + \alpha^*\right) = \ell_0\sqrt{2}\,\mathrm{Re}\{\alpha\},$$

Thus, the real part of α is connected to the expectation value of the position operator

$$\mathrm{Re}\{\alpha\} = \frac{\langle\hat{x}\rangle}{\sqrt{2}\,\ell_0}.$$

Now, for the momentum operator

$$\hat{p} = \frac{i\hbar}{\sqrt{2}\ell_0}(\hat{a}^\dagger - \hat{a}),$$

the expectation value in the coherent state is:

$$\begin{aligned}\langle\alpha|\hat{p}|\alpha\rangle &= \frac{i\,\hbar}{\sqrt{2}\,\ell_0}\langle\alpha|\left(\hat{a}^\dagger - \hat{a}\right)|\alpha\rangle \\ &= -\frac{i\,\hbar}{\sqrt{2}\,\ell_0}\left(\alpha - \alpha^*\right) \\ &= -\frac{i\,\hbar}{\sqrt{2}\,\ell_0}\left(2\,i\,\mathrm{Im}(\alpha)\right) \\ &= \frac{\hbar\sqrt{2}}{\ell_0}\mathrm{Im}(\alpha),\end{aligned}$$

and thus:

$$\mathrm{Im}\{\alpha\} = \frac{\ell_0\,\langle\hat{p}\rangle}{\hbar\sqrt{2}}.$$

(g) Use your result from the previous question and show that:

$$|\alpha\rangle = \exp\left(-\frac{i\,\hat{p}\,\langle x\rangle}{\hbar} + \frac{i\,\langle p\rangle\,\hat{x}}{\hbar}\right)|0\rangle. \tag{3.10}$$

We have found that the complex α can be expressed in terms of the expectation values of position and momentum operators, i.e.

$$\alpha = \frac{\langle x\rangle}{\ell_0\sqrt{2}} + i\frac{\ell_0\,\langle p\rangle}{\hbar\sqrt{2}}.$$

Also, the ladder operators can be expressed in terms of the position and momentum operators as follows:

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\Big[\frac{\hat{x}}{\ell_0} + \frac{\ell_0 \hat{p}}{i\hbar}\Big], \quad \hat{a} = \frac{1}{\sqrt{2}}\Big[\frac{\hat{x}}{\ell_0} - \frac{\ell_0 \hat{p}}{i\hbar}\Big].$$

Using the above results, we can show by simple algebraic manipulation that

$$\alpha \hat{a}^\dagger - \alpha^* \hat{a} = \frac{i\,\hat{p}\,\langle x\rangle}{\hbar} + \frac{i\,\langle p\rangle\,\hat{x}}{\hbar}$$

and thus we obtain the desired result.

(h) Considering the harmonic oscillator, evolve the coherent state in time, and show that $|\alpha(t)\rangle$ remains an eigenstate of $\hat{a}$, and the eigenvalue evolves in time:

$$\alpha(t) \;=\; e^{-i\omega t}\,\alpha.$$

Hence a coherent state stays coherent, and continues to minimize the uncertainty product.

We apply the time-evolution operator on the coherent state

$$|\alpha(t)\rangle = U(t)\,|\alpha\rangle = e^{-iHt/\hbar}$$

where $H = \hbar\omega(N + \frac{1}{2})$ is the Hamiltonian of the harmonic oscillator. We use the expansion of the coherent state in terms of the energy eigenstates to find the action of the time-evolution operator on the coherent state:

$$\begin{aligned} |\alpha(t)\rangle &= e^{-i\omega t/2} e^{-i\hat{N}\omega t} \sum_{n=0}^{\infty} c_n\,|n\rangle \\ &= e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} c_n\,|n\rangle\,. \end{aligned}$$

To show that this state remains an eigenstate of $\hat{a}$,

$$\begin{aligned} \hat{a}\,|\alpha(t)\rangle &= e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} c_n a\,|n\rangle \\ &= e^{-i\omega t/2} \sum_{n=1}^{\infty} e^{-in\omega t} c_n \sqrt{n}\,|n-1\rangle\,, \end{aligned}$$

and we have used $a\,|n\rangle = \sqrt{n}\,|n-1\rangle$. Notice that the sum now runs from $n = 1$ instead of $n = 0$, since the action of the lowering operator to $|0\rangle$ gives zero. We now use the explicit form of the coefficients c_n and proceed as follows:

$$\begin{aligned} \hat{a}\,|\alpha(t)\rangle &= e^{-i\omega t/2} \sum_{n=1}^{\infty} e^{-in\omega t} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n}\,|n-1\rangle \\ &= e^{-i\omega t/2} \alpha e^{-i\omega t} \sum_{n=1}^{\infty} e^{-i(n-1)\omega t} \frac{\alpha^{(n-1)}}{\sqrt{(n-1)!}}\,|n-1\rangle \\ &= \alpha e^{-i\omega t} e^{-i\omega t/2} \sum_{m=0}^{\infty} e^{-im\omega t} \frac{\alpha^m}{\sqrt{m!}}\,|m\rangle \\ &= \alpha e^{-i\omega t}\,|\alpha(t)\rangle\,, \end{aligned}$$

thus showing that indeed the time-evolved coherent state remains an eigenstate of the lowering operator.

(i) Is the ground state of the harmonic oscillator a coherent state? If so, what is the eigenvalue?

The ground state is a coherent state, an eigenstate of the lowering operator with $\alpha = 0$

$$a\,|0\rangle = 0\,|0\rangle\,.$$

Remark: On physical grounds, coherent states are indeed special quantum states arising from the harmonic oscillator and they are the "most classical" quantum states, due to having many classical-like properties. They are found for example in quantum optics (where they can be used to describe laser light) and condensed matter, where they are often used to describe collective behavior such as in Bose-Einstein condensation, superconductivity and superfluidity.

4 The Propagator in Quantum Mechanics

In quantum mechanics, the propagator is a fundamental object that describes how a particle's quantum state evolves from one point in space and time to another. It gives the amplitude for a particle to travel from position x' at time t_0 to position x at time t, and essentially encodes the full dynamics of the system. It is defined as:

$$\mathcal{K}(x,\,x';\,t-t_0)\;\equiv\;\langle x|e^{-\frac{i}{\hbar}(t-t_0)\,\hat{H}}|x'\rangle. \tag{4.1}$$

In any given system, the propagator depends only on the potential and its independent of the initial state. As we will show in this exercise, the propagator can be constructed once the energy eigenfunctions and their eigenvalues are given.

The propagator is central to both the path integral formulation and the Schrödinger picture, linking initial and final states via an integral kernel that "propagates" the wavefunction forward in time.

(a) Show that, when the system (i.e. the Hamiltonian) is invariant under space translations $x \to x + \alpha$ (as for instance in the free-particle case), the propagator has the property

$$\mathcal{K}(x,\,x';\,t-t_0)\;=\;\mathcal{K}(x-x';\,t-t_0).$$

Space translations are expressed through the action of an operator as follows:

$$\langle x|e^{\frac{i}{\hbar}\alpha\cdot\hat{p}}\;=\;\langle x+\alpha|.$$

Space-translation invariance holds if

$$[\hat{p},\,\hat{H}]\;=\;0\quad\Longrightarrow\quad e^{\frac{i}{\hbar}\alpha\cdot\hat{p}}\,\hat{H}\,e^{-\frac{i}{\hbar}\alpha\cdot\hat{p}}\;=\;\hat{H},$$

which also implies that

$$e^{\frac{i}{\hbar}\alpha\cdot\hat{p}}\, e^{-\frac{i}{\hbar}(t-t_0)\,\hat{H}}\, e^{-\frac{i}{\hbar}\alpha\cdot\hat{p}} \;=\; e^{-\frac{i}{\hbar}(t-t_0)\,\hat{H}}.$$

Thus we have

$$\mathcal{K}(x,\, x';\, t-t_0) \;=\; \langle x+\alpha \,|\, e^{-\frac{i}{\hbar}(t-t_0)\,\hat{H}} \,|\, x'+\alpha\rangle \;=\; \mathcal{K}\big(x+\alpha,\; x'+\alpha;\; t-t_0\big).$$

which clearly implies that the propagator can only be a function of the difference $x - x'$.

(b) Show that the propagator can be expressed in terms of the eigenstates $\psi_E(x)$ of the Hamiltonian:

$$\mathcal{K}(x,\, x';\, t-t_0) = \sum_E e^{-i(t-t_0)E/\hbar}\psi_E(x)\psi_E^*(x').$$

We consider the definiton of the propagator as given in the beginning of this exercise. Using the completeness relation for the eigenstates of the Hamiltonian

$$\mathbb{1} = \sum_E |E\rangle\,\langle E|$$

we have:

$$\mathcal{K}(x, x'; t-t_0) = \sum_E \langle x| e^{-\frac{i}{\hbar}(t-t_0)\,\hat{H}} |E\rangle\,\langle E|x'\rangle\,.$$

We use the notation $\psi_E(x) = \langle E|x\rangle$ for the wavefunctions. We also use the fact that the time evolution operator acting on one of the eigenstates of the system provides the usual phase factor, and thus:

$$\mathcal{K}(x, x'; t-t_0) = \sum_E e^{-\frac{i}{\hbar}(t-t_0)E}\psi_E(x)\psi_E^*(x').$$

(c) Show that when the energy eigenfunctions are real, i.e. $\psi_E(x) = \psi_E^*(x)$ (as in the harmonic oscillator), the propagator has the property

$$\mathcal{K}(x,\, x';\, t-t_0) \;=\; \mathcal{K}(x',\, x;\, t-t_0).$$

Consider the propagator as obtained from the previous question. With real eigenstates, we obtain

$$\mathcal{K}(x, x';\, t-t_0) = \sum_E e^{-\frac{i}{\hbar}(t-t_0)\,E}\psi_E(x)\psi_E(x').$$

It is evident that the order of x, x' does not matter, and thus

$$\mathcal{K}(x,\, x';\, t-t_0) = \mathcal{K}(x',\, x;\, t-t_0).$$

(d) Show that when the energy eigenfunctions are also parity eigenfunctions (i.e. even or odd functions), the propagator has the property

$$\mathcal{K}(x,\, x';\, t-t_0) \;=\; \mathcal{K}\big(-x,\, -x';\, t-t_0\big). \tag{4.2}$$

This can be shown by using the result of Question (b),

$$\begin{aligned}\mathcal{K}(-x,\, -x';\, t-t_0) &= \sum_E \psi_E(-x)\, e^{-\frac{i}{\hbar}(t-t_0)\,E}\, \psi_E^*(-x') \\ &= \sum_E (\pm)^2\, \psi_E(x)\, e^{-\frac{i}{\hbar}(t-t_0)\,E}\, \psi_E^*(x') \\ &= \mathcal{K}(x,\, x';\, t-t_0).\end{aligned}$$

We have used the fact that the energy eigenstates $\psi_E(x)$ have either odd $\psi_E(-x) = -\psi_E(x)$ or even parity $\psi_E(-x) = +\psi_E(x)$.

(e) Show that we always have the property

$$\mathcal{K}(x,\, x';\, t-t_0) \;=\; \mathcal{K}^*\big(x',\, x;\, -t+t_0\big).$$

Again, this can be shown by using the result of Question (b),

$$\begin{aligned}\mathcal{K}(x,\; x';\, t-t_0) &= \sum_E \psi_E(x)\, e^{-\frac{i}{\hbar}(t-t_0)\,E}\, \psi_E^*(x') \\ &= \Big[\sum_E \psi_E^*(x)\, e^{-\frac{i}{\hbar}(t_0-t)\,E}\, \psi_E(x')\Big]^* \\ &= \mathcal{K}^*\big(x',\, x;\; t_0-t\big).\end{aligned}$$

(f) Show that the final state can be obtained by using the propagator

$$\psi(x,t) = \int dx'\, \mathcal{K}(x,x';t-t_0)\psi(x',t_0). \tag{4.3}$$

The final state can be given by considering the time evolution of the initial state through the time-evolution operator,

$$|\psi(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}\, |\psi(t_0)\rangle\,.$$

By taking the bra $\langle x|$ on both sides and using the completeness relation for the position representation in the RHS, we have

$$\langle x|\psi(t)\rangle = \int dx'\;\langle x|\, e^{-i\hat{H}(t-t_0)/\hbar}\, |x'\rangle\, \langle x'|\psi(t_0)\rangle$$

We identify $\langle x|\, e^{-i\hat{H}(t-t_0)/\hbar}\, |x'\rangle$ as the propagator $\mathcal{K}(x,x';t-t_0)$ and $\langle x|\psi(t)\rangle$ as the spatial wavefunction, thus:

$$\psi(x,t) = \int dx'\, \mathcal{K}(x,x';t-t_0)\psi(x',t_0).$$

(g) Calculate the propagator of a free particle that moves in one dimension. Show that it is proportional to the exponential of the classical action

$$S \equiv \int dt\, L,$$

defined as the integral of the Lagrangian for a free classical particle starting from the point x at time t_0 and ending at the point x' at time t. For a free particle the Lagrangian coincides with the kinetic energy. Verify also that in the limit $t \to t_0$ we have

$$\mathcal{K}_0(x - x';\, 0) = \delta(x - x'). \tag{4.4}$$

Hint: Consider

$$\mathcal{K}(x,\, x';\, t - t_0) \equiv \langle x| e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} |x'\rangle, \tag{4.5}$$

and use the resolution of identity of the momentum representation.

The propagator is

$$\mathcal{K}_0(x, x';\, t - t_0) = \int dp\, \langle x| e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\, |p\rangle\, \langle p|\, x'\rangle.$$

Since the Hamiltonian of the free particle is simply $H = p^2/2m$, thus the time-evolution operator acting on a momentum eigenket will give the usual phase,

$$\mathcal{K}_0(x, x';\, t - t_0) = \int dp\, e^{-i(t-t_0)\frac{p^2}{2m\hbar}}\, \langle x|p\rangle\, \langle p|\, x'\rangle.$$

Now recall the eigenstates of the momentum operator in the position representation take the form of a plane wave, i.e.

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}},$$

and thus the propagator becomes:

$$\begin{aligned}\mathcal{K}_0(x, x';\, t - t_0) &= \frac{1}{2\pi\hbar}\int dp\, e^{-i(t-t_0)\frac{p^2}{2m\hbar}}\, e^{ipx/\hbar} e^{-ipx'/\hbar} \\ &= \frac{1}{2\pi\hbar}\int dp\, \exp\left\{ + \frac{i}{\hbar}(x - x')p - \frac{i}{2m\hbar}(t - t_0)p^2 \right\}.\end{aligned}$$

We now use the hint provided

$$\int_{-\infty}^{+\infty} \exp\left[-\left(a\, x^2 + b\, x + c\right)\right] dx = \sqrt{\frac{\pi}{a}}\, \exp\left(\frac{b^2}{4\,a} - c\right).$$

where $a = i(t - t_0)/(2m\hbar)$, $b = -i(x - x')/\hbar$ and $c = 0$. Thus, the propagator becomes:

$$\mathcal{K}_0(x, x';\, t - t_0) = \left[\frac{m}{2\pi\hbar i(t - t_0)}\right]^{1/2} \exp\left\{ i\frac{m(x - x')^2}{2\hbar(t - t_0)} \right\}.$$

The exponent can be written as $iS/\hbar$ where S is the classical action. A simple calculation indeed confirms that this corresponds to the classical action, since:

$$S = \int_{t_0}^{t} dt\, \frac{m\,v^2}{2} = (t - t_0)\,\frac{m}{2}\left(\frac{x - x'}{t - t_0}\right)^2 = \frac{m\,(x - x')^2}{2\,(t - t_0)}.$$

In order to consider the limit $t \to t_0$, it is helpful to insert a small imaginary part into the time variable, according to

$$t \;\to\; t \;-\; i\,\epsilon.$$

Then, we can safely take $t = t_0$ and consider $\epsilon \to 0$. We get

$$\mathcal{K}_0(x - x';\, 0) = \lim_{\epsilon\to 0}\left\{\left[\frac{m}{2\pi\hbar\varepsilon}\right]^{1/2} \exp\left\{-\frac{m(x - x')^2}{2\hbar\varepsilon}\right\}\right\} \;=\; \delta\big(x - x'\big).$$

For the last step we used the well-known Gaussian representation of the delta function,

$$\delta(x) = \lim_{\epsilon\to 0}\big(\epsilon\,\pi\big)^{-\frac{1}{2}}\exp\big[-x^2/\,\epsilon\big].$$

(h) Consider the case of a free particle initially in the plane-wave state

$$\psi(x, t_0) = \frac{1}{\sqrt{2\pi}}\exp\!\Big(ikx - i\,\frac{\hbar\,k^2}{2\,m}\,t_0\Big) \tag{4.6}$$

and, using the expression for the free propagator, find the time-evolved state $\psi(x, t)$.

The time-evolved state is obtained by

$$\psi(x, t) = \int dx'\,\mathcal{K}(x, x'; t - t_0)\psi(x', t_0),$$

where the propagator corresponds to that of a free particle, derived in the previous question. Using the initial state given, we have:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}}\int dx'\, A(t)e^{iB(t)(x - x')^2}e^{ikx'}e^{-iC(t_0)},$$

where we have defined (short-hand notation):

$$A(t) = \left[\frac{m}{2\pi\hbar i(t - t_0)}\right]^{1/2}, \quad B(t) = \frac{m}{2\hbar(t - t_0)}, \quad C(t_0) = \frac{\hbar\,k^2}{2\,m}\,t_0.$$

Re-arranging the above equation, we have:

$$\psi(x, t) = \frac{A(t)}{\sqrt{2\pi}}e^{-iC(t_0)}\int dx'\, e^{iB(t)(x - x')^2}e^{ikx'},$$

and changing variables $x - x' = z$, we find:

$$\psi(x,t) = \frac{A(t)}{\sqrt{2\pi}} e^{-iC(t_0)} e^{ikx} \int dz\, e^{iB(t)z^2 - ikz}.$$

We are left with a Gaussian integral, which is of the following form

$$\int_{-\infty}^{+\infty} \exp\left[-\left(a\,x^2 + b\,x + c\right)\right] dx = \sqrt{\frac{\pi}{a}}\ \exp\left(\frac{b^2}{4\,a} - c\right).$$

where $a = B(t)/i$, $b = ik$ and $c = 0$. Thus, using this identity, we find the time-evolved state

$$\psi(x,t) = \frac{A(t)}{\sqrt{2\pi}} e^{-iC(t_0)} e^{ikx} \sqrt{\frac{i\pi}{B(t)}} e^{-\frac{ik^2}{4B(t)}},$$

which further simplifies to:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{ikx - i\frac{\hbar^2 k^2}{2m} t/\hbar}. \tag{4.7}$$