Homework 2

Version as of Nov 7, check for updates

Due date for HW2 is **Wed, Nov 20, 20:00.**

Rules

[1] File Format: Submit only one PDF file. The filename must follow the format: Firstname_Lastname_homework2.pdf.

[2] Submission Method: Using LaTeX or a handwriting app on an iPad is strongly recommended. If you want to submit handwritten paperwork, it must be scanned by a printer and saved as a PDF pictures converted to PDF are not acceptable.

[3]Answer Order: Answer the questions in the same order they are listed. Do not change the order or mix them up.

[4] Highlighting Answers: Underline each final answer clearly.

[5] QuTiP Outputs: When using QuTiP, include only a screenshot of the final result. Do not include the entire code.

[6] Legibility of Handwritten Figures: Handwritten figures must be clear and easy to read. Illegible figures will result in a loss of points.

[7] Deadline: Late submissions will not be accepted under any circumstances.

Each exercise is worth 1 point.
Extra point for each error reported on the forum (minus trivial typos).

A. Introduction: classical vs. quantum oscillator models

Classical model

The classical Hamiltonian function for a harmonic oscillator is given by the following expression:

$$H(x,p) = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} = \omega\left[x\sqrt{\frac{m\omega}{2}} + i\frac{p}{\sqrt{2m\omega}}\right]\left[x\sqrt{\frac{m\omega}{2}} - i\frac{p}{\sqrt{2m\omega}}\right], \tag{1}$$

where x is position, m is mass, p is momentum, and ω is the resonance frequency (we eliminated the spring constant $k = m\omega^2$). We can replace position and momentum variables with linear combinations of position and momentum, $A = \left[x\sqrt{\frac{m\omega}{2}} + i\frac{p}{\sqrt{2m\omega}}\right]$ and $A^* = \left[x\sqrt{\frac{m\omega}{2}} - i\frac{p}{\sqrt{2m\omega}}\right]$, and rewrite the Hamiltonian function as

$$H(A, A^*) = \omega A A^* = \omega A^* A. \tag{2}$$

With these new variables, the equations of (Newtonian) motion are particularly simple:

$$\dot{A} = -i\omega A. \tag{3}$$

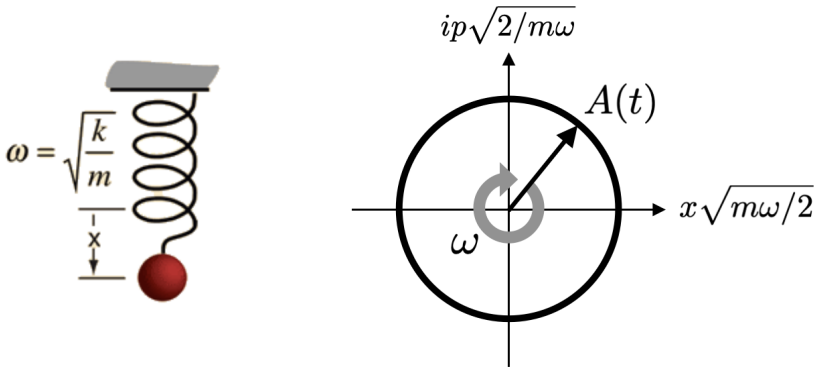

Figure 1: Schematic of a harmonic oscillator and its classical motion. The vector $A(t)$ rotates in the complex plane at a rate ω. Presented this way, one may argue that the harmonic oscillator motion is the simplest possible type of motion.

The solution is $A(t) = A(t = 0)\exp(-i\omega t)$. The complex number A is a vector in the Re-Im plane and it just rotates at an angular frequency ω starting from its initial value $A(t = 0)$. The conjugate vector A^* does the same except rotating in the opposite direction. At any given time we know $A(t)$ and $A^*(t)$ from which we get position $x(t) = (A(t) + A(t)^*)\sqrt{\frac{1}{2m\omega}}$ and and momentum $p(t) = i(A(t)^* - A(t))\sqrt{\frac{m\omega}{2}}$. The length $|A|$ stays constant, which makes sense, because $|A|^2 = A^*A$ is proportional to the oscillator's total energy. The total energy stays the same, periodically redistributing between the potential energy $U(x) = m\omega^2 x^2/2$ and the kinetic energy $p^2/2m$.

Quantum model

For a quantum description, we first have to come up with a vector space to define the oscillators quantum states $|\Psi\rangle$ by analogy with qubits. It can be a bit more tricky, though, since we might need more than two basis vectors. Next, we need to figure out how the operators such as $\hat{x}$ and $\hat{p}$ act on $|\Psi\rangle$. Next, we would set up the Schrodinger's equation

$$\partial|\Psi(t)\rangle/\partial t = (-i/\hbar)\hat{H}(\hat{x}, \hat{p})|\Psi\rangle, \tag{4}$$

solve for $|\Psi(t)\rangle$, and use it to learn everything quantum mechanics allow us to know about the motion of a quantum harmonic oscillator.

How do we start? Let's recall a general property of quantum evolution for the mean values of observables. We already encountered this with qubits:

$$\partial\langle\hat{x}\rangle/\partial t = (-i/\hbar)\langle[\hat{x}, \hat{H}]\rangle = (-i/\hbar)\langle\hat{x}\hat{H} - \hat{H}\hat{x}\rangle, \tag{5}$$

where $\langle ...\rangle = \langle\Psi(t)|...|\Psi(t)\rangle$. Moreover, we expect that the mean values of quantum observables agree with classical mechanics, whenever possible. Classically, we have $\dot{x} = p/m$, so we'd better satisfy $\partial\langle\hat{x}\rangle/\partial t = \langle\hat{p}\rangle/m$. Since $\Psi(t = 0)$ can be chosen arbitrary, the only reasonable option to match the two mean values would be to match the corresponding operators. That is operators $\hat{x}$ and $\hat{p}$ must be related in such a way that $[\hat{x}, \hat{H}] = [\hat{x}, \hat{p}^2/2m] = (+i\hbar) \times \hat{p}/m$. This is equivalent to a commutation relation:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \tag{6}$$

So, we have not yet defined the vector space for a harmonic oscillator, but we already know the commutation relation between momentum and position operators! Without a

basis, we cannot define the matrices for such operators. In fact, one may be puzzled by the mathematical meaning of $\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$: the l.h.s. is an operator, the r.h.s. is a (complex) number. What this means is for any oscillator state $|\Psi\rangle$, we get $(\hat{x}\hat{p} - \hat{p}\hat{x})|\Psi\rangle = i\hbar|\Psi\rangle$.

By analogy with the classical model, we introduce the "ladder" operators (the ladder will come in soon) $\hat{a}$ and $\hat{a}^\dagger$: $\hat{a} = \frac{1}{2}(\hat{x}/x_0) + \frac{1}{2}i(\hat{p}/p_0)$ and $\hat{a}^\dagger = \frac{1}{2}(\hat{x}/x_0) - \frac{1}{2}i(\hat{p}/p_0)$:

$$\hat{x} = x_0(\hat{a} + \hat{a}^\dagger) \tag{7}$$

$$\hat{p} = -ip_0(\hat{a} - \hat{a}^\dagger) \tag{8}$$

$$[a, a^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \tag{9}$$

where $x_0 = \sqrt{\hbar/2m\omega}$ and $p_0 = \sqrt{\hbar m\omega/2}$ (it's helpful to remember that $x_0 p_0 = \hbar/2$). The commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$ follows directly from $[\hat{x}, \hat{p}] = i\hbar$. The Hamiltonian operator becomes

$$\hat{H} = \hbar\omega a^\dagger a + \frac{1}{2}\hbar\omega \tag{10}$$

So far, this way of writing the Hamiltonian does not buy us anything until we learn some more about the way operator $\hat{a}$ works. Curiously, the operator $\hat{a}$ is neither hermitian ($\hat{a}^\dagger \neq \hat{a}$) nor unitary ($\hat{a}^\dagger a \neq \hat{a}\hat{a}^\dagger$). Nevertheless, this operator is going to be quite useful. The operator $\hat{a}^\dagger a$ is called the "number" operator, it is hermitian, since it represents an observable related to the oscillator's energy.

Energy eigenstates (Fock states) basis

We can construct the vector space for a quantum harmonic oscillator using the eigenstates of the Hamiltonian operator, also called energy eigenstates or Fock states. We stick to Dirac notations and denote the state $|E\rangle$ as the energy eigenstate of $\hat{H}$ with eigenvalue E, that is $\hat{H}|E\rangle = E|E\rangle$. To start our construction, let us find out how the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ act on an energy eigenstate $|E\rangle$. What can we learn about state $\hat{a}^\dagger|E\rangle$? Check this out:

$$\hat{H}\big(\hat{a}^\dagger|E\rangle\big) = \hbar\omega(\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger/2)|E\rangle = \hbar\omega\hat{a}^\dagger(\hat{a}^\dagger\hat{a} + 1 + 1/2)|E\rangle = \hat{a}^\dagger\hat{H}|E\rangle + \hbar\omega\hat{a}^\dagger|E\rangle =$$
$$= (E + \hbar\omega)\big(\hat{a}^\dagger|E\rangle\big)$$

Thus, for any eigenstate $|E\rangle$ of $\hat{H}$ with eigenvalue E, the state $\hat{a}^\dagger|E\rangle$ is also an eigenstate of $\hat{H}$ but with a higher eigenvalue (energy) $E + \hbar\omega$. What state would be $\hat{a}|E\rangle$ then?

$$\hat{H}\big(\hat{a}|E\rangle\big) = \hbar\omega(\hat{a}^\dagger\hat{a}\hat{a} + \hat{a}/2)|E\rangle = \hbar\omega(\hat{a}\hat{a}^\dagger - 1 + 1/2)\hat{a}|E\rangle = \hat{a}\hat{H}|E\rangle - \hbar\omega\hat{a}|E\rangle =$$
$$= (E - \hbar\omega)\big(\hat{a}|E\rangle\big)$$

Thus, for any energy eigenstate $|E\rangle$ with an eigenvalue E, the state $\hat{a}|E\rangle$ is also an energy eigenstate but with a lower eigenvalue (energy) $E - \hbar\omega$.

The ground state. Applying $\hat{a}$ operator twice, we find that state $\hat{a}\big(\hat{a}|E\rangle\big)$ is also an eigenstate of $\hat{H}$ with eigenvalue $E - 2\hbar\omega$, and so on. Eventually, we will reach a special eigenstate $|0\rangle$, also called "ground" state, which corresponds to the lowest possible eigenvalue of $\hat{H}$ given by E_0 – the lowest possible energy that a quantum oscillator can have. How do we organize that there are no eigenstates of $\hat{H}$ with eigenvalues lower than E_0? The only way is to satisfy

$$\hat{a}|0\rangle = 0 \tag{11}$$

That is, applying operator $\hat{a}$ to the ground state ket $|0\rangle$ does not produce any new ket but rather produces what's usually called a null-vector in linear algebra. Imagine $\hat{a}$ represented by some matrix and $|0\rangle$ is some column vector (we'll get there), then multiplying the column by the matrix gives a column all filled with zeros.

The ground state energy. Let's find out this lowest possible (ground state) energy E_0. Given that $\hat{a}^\dagger\big(\hat{a}|0\rangle\big) = 0$ and $\hat{H}|0\rangle = E_0|0\rangle$, we get

$$E_0 = \langle 0|\hat{H}|0\rangle = \hbar\omega\langle 0|\hat{a}^\dagger\hat{a}|0\rangle + \frac{1}{2}\hbar\omega\langle 0|0\rangle = \frac{1}{2}\hbar\omega. \tag{12}$$

Unlike classical oscillators, the lowest possible energy of a quantum oscillator is not zero. A quantum oscillator apparently just can't stay still! The motion associated with the ground state energy $\hbar\omega/2$ is called "zero-point" motion. How cool is that?

The first excited state. The next lowest energy eigenstate $|1\rangle$ must be given by $|1\rangle = C_1\hat{a}^\dagger|0\rangle$ and have energy $E_1 = E_0 + \hbar\omega$. Can it be that there is some other energy eigenstate $|E'\rangle$ with a lower eigenvalue $E' < E_0 + \hbar\omega$? No, because then a state $\hat{a}|E'\rangle$ would be an eigenstate with energy less than E_0, which is impossible. The constant C_1 is generally necessary to ensure the normalization $\langle 1|1\rangle = \langle 0|0\rangle = 1$. How do we recover the value of C_1? Recall that $\big(C_1\hat{a}^\dagger|0\rangle\big)^\dagger = C_1^*\langle 0|\hat{a}$, so the normalization condition becomes $1 = \langle 1|1\rangle = |C_1|^2\langle 0|\hat{a}\hat{a}^\dagger|0\rangle$. We also know that $\langle 0|\hat{a}\hat{a}^\dagger|0\rangle = \langle 0|1 + \hat{a}^\dagger\hat{a}|0\rangle = \langle 0|0\rangle = 1$, so we may set $C_1 = 1$ and the final result is:

$$|1\rangle = \hat{a}^\dagger|0\rangle \tag{13}$$

$$\hat{H}|1\rangle = (E_0 + \hbar\omega)|1\rangle = \frac{3}{2}\hbar\omega|1\rangle \tag{14}$$

Complete energy eigenstates basis. We can proceed creating higher energy eigenstates by applying $\hat{a}^\dagger$ operator to the ground state n times. Consider the n-th lowest energy eigenstate $|n\rangle$ with eigenvalue $E_n = \frac{1}{2}\hbar\omega + n\hbar\omega$. This is what we know already about it:

$$|n\rangle = C_n\hat{a}^\dagger|n-1\rangle = C_nC_{n-1}(\hat{a}^\dagger)^2|n-2\rangle = C_nC_{n-1}C_{n-2}(\hat{a}^\dagger)^3|n-3\rangle = ... \tag{15}$$

$$\hat{H}|n\rangle = \hbar\omega(n + 1/2)|n\rangle \tag{16}$$

To find the normalization constant, we notice that $\langle n|\hat{a}^\dagger\hat{a}|n\rangle = n$ and $1 = \langle n|n\rangle = \langle n-1|\hat{a}C_n^*C_n\hat{a}^\dagger|n-1\rangle = |C_n|^2\langle n-1|1 + \hat{a}^\dagger\hat{a}|n-1\rangle = |C_n|^2 n$, that is $C_n = 1/\sqrt{n}$. Also notice that $\hat{a}\big(\hat{a}^\dagger|n-1\rangle\big) = \sqrt{n}\hat{a}|n\rangle$ but also $\hat{a}\big(\hat{a}^\dagger|n-1\rangle\big) = (1 + \hat{a}^\dagger\hat{a})|n-1\rangle = n|n-1\rangle$, which finally leads us to:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \tag{17}$$

$$\hat{a}^\dagger|n-1\rangle = \sqrt{n}|n\rangle \tag{18}$$

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \tag{19}$$

Our construction of the quantum harmonic oscillator vector space is complete! We have a (infinite by countable) set of orthonormal kets $|n\rangle$, $n = 0, 1, 2, ..$ which are the energy eigenstates (a.k.a. Fock states), we know how the ladder operators $\hat{a}$ **(the lowering operator)** and $\hat{a}^\dagger$ **(the raising operator)** act in this basis, and we can express operators

of physical quantities, such as energy, position, and momentum via the ladder operators.

Summary. A quantum harmonic oscillator can only have discrete values of energy $E_n = \hbar\omega(n + 1/2)$. The quantum of energy $\hbar\omega$ is proportional to the oscillator's classical frequency ω and we need the Planck's constant $\hbar$ to relate frequency and energy. The lowest possible energy is non-zero but $\hbar\omega/2$. By analogy with qubits, any state $|\Psi\rangle$ an oscillator can be written as a superposition of its energy eigenstates (Fock states):

$$|\Psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle + \psi_2|2\rangle + ... = \sum_{n=0}^{\infty} \psi_n|n\rangle \tag{20}$$

where ψ_0, ψ_1, ψ_2, etc. are complex numbers (amplitudes). Just like in the case of qubits, we are allowed to query a quantum oscillator in some state $|\Psi\rangle$ "what is your energy?" The reading on the "energy meter" would be $\hbar\omega(n+1/2)$, $n = 0, 1, 2, ...$, with a probability $|\langle n|\Psi\rangle|^2 = |\psi_n|^2$. Following such a query (the quantum measurement), the oscillator is initialized in a specific energy eigenstate, corresponding to the eigenvalue indicated by the meter. Repeated measurements would thus copy the first measurement result. To keep the total probability of all possible measurement outcomes unity, we require $\sum_n |\psi_n|^2 = 1$. The global phase factor does not matter and can be removed: for example, ψ_0 can always be chosen a real number). For better or worse, there is no Bloch sphere for oscillators, because we are no longer restricted to two basis states (the north pole and the south pole).

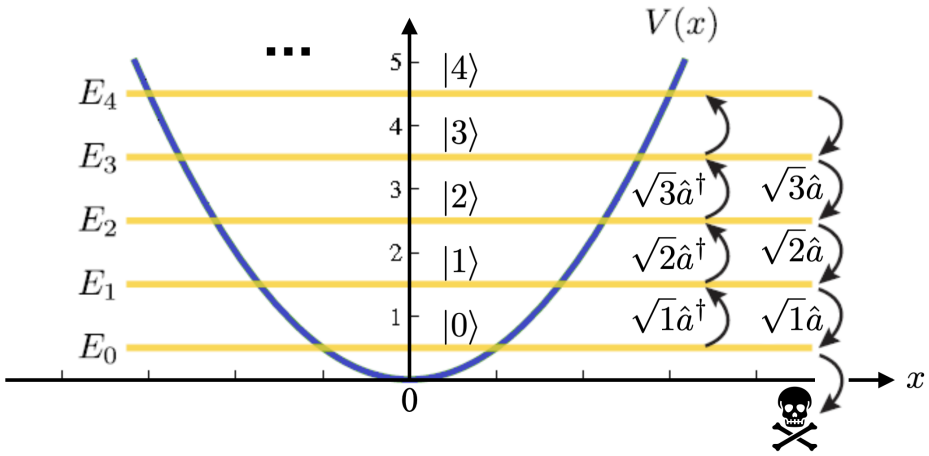

Figure 2: Illustration of the quantum harmonic oscillator energy eigenstates and the ladder operators. There is a minimal energy state, called the ground state $|0\rangle$, but there is no maximal energy state. The function $V(x)$ represents the potential energy, in our case given by $V(x) = m\omega^2x^2/2$.

The Hamiltonian operator in Dirac notations can be written as

$$\hat{H}/\hbar\omega = \frac{1}{2}|0\rangle\langle 0| + \frac{3}{2}|1\rangle\langle 1| + \frac{5}{2}|2\rangle\langle 2| + \frac{7}{2}|3\rangle\langle 3| + ... \tag{21}$$

The time evolution is given by the unitary operator $|\Psi(t)\rangle = \hat{U}(t)|\Psi(t=0)\rangle$:

$$\hat{U}(t) = \exp(-i\hat{H}t/\hbar) = \exp(-i\omega t\hat{a}^\dagger\hat{a}) \tag{22}$$

(yes, we removed the global phase factor due to the $\hbar\omega/2$-term). In analogy with qubits, the time-evolution is the simplest in the energy eigenstates basis:

$$|\Psi(t)\rangle = \exp(-i\omega t\hat{a}^\dagger\hat{a})|\Psi(t=0)\rangle \tag{23}$$

$$|\Psi(t)\rangle = \sum_{n=0}^{\infty}\Big[\psi_n \exp(-in\omega t)\Big]|n\rangle \tag{24}$$

We remind that if $|\Psi(t=0)\rangle$ is one of the Fock states, then it does not really evolve in time aside from being multiplied by the phase factor.

Exercise 1: We are not yet in a position to discuss the outcome of instantaneous measurements of position $\hat{x}$ or momentum $\hat{p}$ observables, like we did with the qubit Pauli operators. However, we can already predict the result of repeating a quantum measurement of $\hat{x}$ and $\hat{p}$ many times (each time starting with the same initial state). Indeed, use Eq. 7 and Eq. 8 and calculate the mean values of $\langle\Psi|\hat{x}|\Psi\rangle$ and $\langle\Psi|\hat{p}|\Psi\rangle$ operators for an oscillator in states $|\Psi\rangle = |0\rangle$ and $|\Psi\rangle = |n\rangle$.

Exercise 2: Calculate $x_{\rm RMS} = \sqrt{\langle\Psi|\hat{x}^2|\Psi\rangle}$ and $p_{\rm RMS} = \sqrt{\langle\Psi|\hat{p}^2|\Psi\rangle}$ for an oscillator in states $|\Psi\rangle = |0\rangle$ and $|\Psi\rangle = |n\rangle$. These two quantities define the "spread" in the values of x and p, reflecting a fundamental quantum-mechanical uncertainty in their values.

Exercise 3: Use the results of the previous exercise and demonstrate that

$$x_{\rm RMS}p_{\rm RMS} \geq \hbar/2 \tag{25}$$

That's the **Heisenberg uncertainty relation**, it tells you that you can't know exact values of position and momentum simultaneously, and the smaller the uncertainty of x, the larger has to be the uncertainty on p.

Exercise 4: We have seen that the ground state energy $E_0 = \hbar\omega/2$ is non-zero. This is in sync with non-zero uncertainties on the values of $x_{\rm RMS}$ and $p_{\rm RMS}$, as if the oscillator indeed can't stop moving. Calculate and compare mean kinetic $\langle 0|\hat{p}^2/2m|0\rangle$ and mean potential $\langle 0|m\omega^2\hat{x}^2/2|0\rangle$ energies of the oscillator in its ground state $|0\rangle$.

The operator $\hat{a}$ is not hermitian, so we cannot query it's instantaneous value. However, we can query operators $\hat{x}$ and $\hat{p}$ (see Eq. 7 and Eq. 8), obtain their mean values, and thereby construct a mean value of $\langle\hat{a}\rangle = \frac{1}{2}\langle\Psi|\hat{x}|\Psi\rangle/x_0 + i\frac{1}{2}\langle\Psi|\hat{p}|\Psi\rangle/p_0$.

Exercise 5: Show by a direct calculation that

$$\partial\langle\hat{a}\rangle/\partial t = -i\omega\langle\hat{a}\rangle \tag{26}$$

$$\partial\langle\hat{a}^\dagger\rangle/\partial t = +i\omega\langle\hat{a}^\dagger\rangle \tag{27}$$

Hint: start by calculating the expectation value $\langle\Psi(t)|\hat{a}|\Psi(t)\rangle$ using Eq. 24. Express the answer in terms of ψ_n amplitudes. Then calculate the time derivative $\partial\langle\Psi(t)|\hat{a}|\Psi(t)\rangle/\partial t$.

Exercise 6: Apply the result of the previous exercise to two cases: $|\Psi(t=0)\rangle = |2\rangle$ and $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. Plot or sketch the time-evolution of $\langle\hat{a}\rangle$ in the 2D plane defined by axis x/x_0 and ip/p_0.

Exercise 7: Plot or sketch the mean energy of the oscillator $\langle\Psi(t)|\hat{H}|\Psi(t)\rangle$ as a function of time for $|\Psi(t=0)\rangle = \sqrt{\frac{1}{3}}|0\rangle + \sqrt{\frac{2}{3}}|n\rangle$ (choose any $n > 0$ you like). Is energy really quantized in a quantum oscillator this time?

B. Coherent states

Consider a special superposition of energy eigenstates, called "coherent" state:

$$|\alpha\rangle = \exp(-|\alpha|^2/2)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{28}$$

A coherent state is parametrized by a complex number α. The state with $\alpha = 0$ is the same state as $|n=0\rangle$, the ground state. The prefactor $\exp(-|\alpha|^2/2)$ is necessary to normalize the state: $\exp(-|\alpha|^2)\sum_n(\alpha\alpha^*)^n/n! = \exp(-|\alpha|^2)\exp(+|\alpha|^2) = 1$. Coherent state is not an energy eigenstate, so it must evolve in time according to Eq. 24. However, the time-evolution is quite simple: we just need to replace α with $\alpha(t)$:

$$|\alpha(t)\rangle = \exp(-|\alpha|^2/2)\sum_{n=0}^{\infty}\frac{\alpha^n(t)}{\sqrt{n!}}|n\rangle, \quad \alpha(t) = \alpha\exp(-i\omega t) \tag{29}$$

In other words, a coherent state at time $t = 0$ remains a coherent state but with a time-evolved parameter $\alpha(t)$. The evolution of $\alpha(t)$ is also simple: $|\alpha|$ remains a constant, while the $\mathrm{Arg}(\alpha)$ changes at a rate ω. The term "coherent" is related to the property that the relative phase between the Fock state amplitudes ψ_n and ψ_{n-1} (see Eq. 20) is the same for all states and is given by $\mathrm{Arg}(\alpha)$.

Exercise 8: Show that a coherent state $|\alpha\rangle$ is an eigenstate of the lowering operator $\hat{a}$ with eigenvalue α:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{30}$$

which gives us a few useful relations:

$$\big(\alpha|\alpha\rangle\big)^\dagger = \alpha^*\langle\alpha| = \big(\hat{a}|\alpha\rangle\big)^\dagger = \langle\alpha|\hat{a}^\dagger \implies \langle\alpha|\hat{a}^\dagger|\alpha\rangle = \alpha^* \tag{31}$$

$$\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = \alpha\alpha^* \tag{32}$$

$$\langle\alpha|\hat{a}\hat{a}^\dagger|\alpha\rangle = \alpha\alpha^* + 1 \tag{33}$$

$$\langle\alpha|\hat{a}^2|\alpha\rangle = \alpha^2 \tag{34}$$

$$\langle\alpha|(\hat{a}^\dagger)^2|\alpha\rangle = (\alpha^*)^2 \tag{35}$$

Interestingly, the eigenvalue α can be any real or complex number and it is not discrete at all. Thus, even though energy eigenvalues of a harmonic oscillator are discrete, there is a continuous nature to it as well!

Exercise 9: Show that the raising operator $\hat{a}^\dagger$ does not have any eigenstates.
Hint: apply $\hat{a}^\dagger$ to a general ket given by Eq. 20 and look for the $|n=0\rangle$ component.

Exercise 10: Using Eq. 30, show that the mean value of energy in a coherent state $|\alpha\rangle$ is given by $\hbar\omega|\alpha|^2 + \hbar\omega/2$. Equivalently, $\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = |\alpha^2|$

Even though the energy eigenvalues are quantized, the mean energy of an oscillator in a coherent state can take any real number (above $\hbar\omega/2$)! As the coherent state evolves in time, the parameter $|\alpha|^2$ stays constant, and so does the mean energy. Phew!

Exercise 11: For an oscillator in a coherent state $|\alpha\rangle$, calculate the variance of the energy, defined by: $E^2_{\text{RMS}} = \langle\alpha|\big(\hat{H} - \langle\alpha|\hat{H}|\alpha\rangle\big)^2|\alpha\rangle = \langle\alpha|\hat{H}^2|\alpha\rangle - \langle\alpha|\hat{H}|\alpha\rangle^2$. The quantity E_{RMS} tells us the fluctuation of the total energy of the oscillator in a coherent state, or the uncertainty in the total number of quanta of energy in the oscillator.

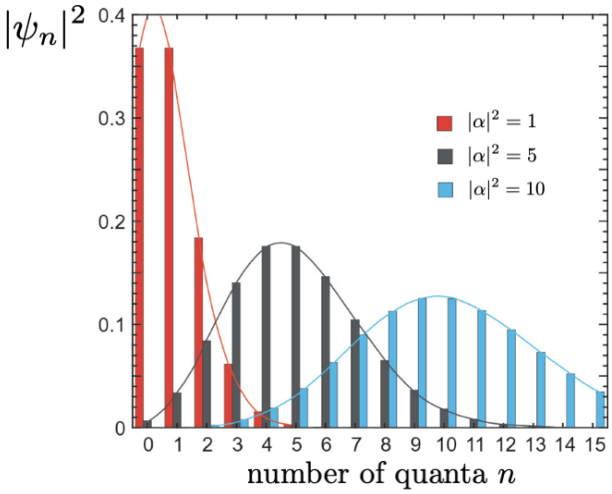

Figure 3: Example distribution of the n-th Fock state probability in a coherent state

Exercise 12: Suppose we query the value of oscillator energy in the same coherent state $|\alpha\rangle$ many-many times and make a histogram of the readings. The probability to read $\hbar\omega(n + 1/2)$ $(n = 0, 1, 2, ...)$ is given by the Poisson distribution

$$P_n = |\langle\alpha|n\rangle|^2 = \exp(-|\alpha|^2) \times |\alpha|^{2n}/n! \tag{36}$$

Sketch the histogram for $|\alpha|^2 = 0, 3.3, 11.7, 100$ (see Fig. 3 as an example). What is the ratio of the mean energy to E_{RMS} for $|\alpha|^2 = 100$?

Exercise 13: Calculate the mean value of $\langle\alpha|\hat{x}|\alpha\rangle$ in a coherent state $|\alpha\rangle$ as well as x_{RMS} given by $x^2_{\text{RMS}} = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$. Does this value change in time?

Exercise 14: Calculate the mean value of $\langle\alpha|\hat{p}|\alpha\rangle$ in a coherent state $|\alpha\rangle$ as well as p_{RMS} given by $p^2_{\text{RMS}} = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2$. Check the product $x_{\text{RMS}} \times p_{\text{RMS}}$? Does it depend on the value of α? (compare to results of Eq. 25)

Exercise 15: Choose $\alpha(t = 0) = 10$ and plot $\langle\hat{x}\rangle$ as a function of time on a computer. Make the thickness of your line equal to x_{RMS}.

The contrast between Fock states and coherent states behavior of a harmonic oscillator reflects the controversial duality of light being simultaneously waves and particles.

C. Displacement operator

We have seen that operator $(\hat{a}^\dagger)^n/\sqrt{n!}$ creates a state $|n\rangle$ from the ground state $|0\rangle$. What would be an operator that turns $|0\rangle$ into a coherent state $|\alpha\rangle$?

Exercise 16: Check the following method of creating coherent state:

$$\exp(-|\alpha|^2/2)\exp(\alpha\hat{a}^\dagger)|0\rangle = |\alpha\rangle \tag{37}$$

$$\exp(\alpha^*\hat{a})|0\rangle = |0\rangle \tag{38}$$

No trick here, just use the Taylor series of the matrix exponent and the definition Eq. 28

In dealing with matrix exponent of Pauli operators, I always encouraged you to use the basis of eigenstates of the operator inside the exponent. For example, the time-evolution operator $\exp(-i\hat{a}^\dagger\hat{a}\omega t)$ applied to a state $|n\rangle$ is equivalent to multiplying it by a phase-factor $\exp(-in\omega t)$, simple! However, dealing with $\exp(\hat{a}^\dagger)$ that way won't work, because $\hat{a}^\dagger$ has no eigenvectors! So we are going to need a couple of new tricks.

Baker Campbell Hausdorff (BCH) formula. Consider operators $\hat{A}$ and $\hat{B}$, such that the commutator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = c$, and, importantly, c is just a number. It can be shown (we don't give a proof here) that

$$\exp(\hat{A})\exp(\hat{B}) = \exp(\hat{A}+\hat{B})\exp\Big(\frac{1}{2}[A,B]\Big) \tag{39}$$

Exercise 17: Prove that

$$\exp(-|\alpha|^2/2)\exp(\alpha\hat{a}^\dagger)\exp(-\alpha^*\hat{a}) = \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a}) \tag{40}$$

Hint: use the BCH formula and $[\alpha^*\hat{a}, \alpha\hat{a}^\dagger] = |\alpha|^2$

Next, because $\exp(-\alpha^*\hat{a})|0\rangle = |0\rangle$, we can formulate a better operator for creating a coherent state from the ground state, known as the "displacement" operator:

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle \tag{41}$$

$$\hat{D}(\alpha) = \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a}) \tag{42}$$

Exercise 18: Prove that displacement operator redefined as by Eq. 42 is unitary and that $\hat{D}^{-1}(\alpha) = \hat{D}(-\alpha) = \hat{D}^\dagger(\alpha)$.

Exercise 19: Prove the following commutation relations:

$$\hat{D}^\dagger(\alpha)\hat{a} = (\hat{a}+\alpha)\hat{D}^\dagger(\alpha) \tag{43}$$

$$\hat{D}^\dagger(\alpha)\hat{a}^\dagger = (\hat{a}^\dagger+\alpha^*)\hat{D}^\dagger(\alpha) \tag{44}$$

Hint: apply the two operators in question to an arbitrary coherent state $|\beta\rangle$. Show first that $\hat{D}(\alpha)\hat{D}(\beta) = D(\alpha+\beta)\exp((\alpha\beta^* - \beta\alpha^*)/2)$.

Exercise 20: Show that for a real α (that is $\alpha^* = \alpha$) the displacement operator becomes:

$$\hat{D}(\alpha) = \exp\Big(-i\frac{\hat{p}\times 2\alpha x_0}{\hbar}\Big) \tag{45}$$

The momentum operator generates displacements along the x-axis, which makes sense: in order to change your position you need to have some momentum!

Exercise 21: Prove further that for $\alpha^* = \alpha$

$$\exp\Big(+i\frac{\hat{p}\times 2\alpha x_0}{\hbar}\Big)\hat{x}\exp\Big(-i\frac{\hat{p}\times 2\alpha x_0}{\hbar}\Big) = \hat{x} + 2\alpha x_0 \tag{46}$$

Hint: use the previously proved commutation relations for $\hat{D}, \hat{D}^\dagger$ and $\hat{a}, \hat{a}^\dagger$.

Since the coherent state describes a nearly classical motion of a quantum harmonic oscillator, the action of a displacement operator on the ground state $|0\rangle$ is equivalent to taking a classical oscillator at rest and giving it an initial displacement in $x = x_0(\alpha + \alpha^*)$ and initial momentum $p = -i(\alpha - \alpha^*)$. The larger the value of α, the more accurate is this interpretation. Once displaced, the oscillator begins oscillating, which is equivalent to the rotation of the vector α in the complex plane at a rate ω.

D. Matrix representation of quantum oscillators

Time to learn representing our operators and kets using matrices and column-vectors. In theory, the Fock states basis contains an infinite number of vectors. Computers don't like that. To code reasonable column and raw vectors on a computer we must force the maximal possible number of quanta N_{max} in the oscillator, that is to set $\psi_{n>N_{max}} = 0$. Such a "truncation" is justified if for some reason the evolution of the oscillator does not involve highly excited states.

Let's start with the general state in Eq. 20:

$$|\Psi\rangle = \begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ ...\end{pmatrix}$$

The basis Fock states would be: $|0\rangle = \begin{pmatrix}1\\0\\0\\...\end{pmatrix}$, $|1\rangle = \begin{pmatrix}0\\1\\0\\...\end{pmatrix}$, $|2\rangle = \begin{pmatrix}0\\0\\1\\...\end{pmatrix}$, ...

The inner product is defined as usual:
$\langle\Psi| = |\Psi\rangle^\dagger = (\psi_0^*, \psi_1^*, \psi_2^*, ...)$; $\langle\Psi|\Psi'\rangle = \psi_0^*\psi_0' + \psi_1^*\psi_1' + \psi_2^*\psi_2' + ...$

Exercise 22: Show by explicit matrix multiplication that the identity matrix $\hat{I}$ (ones on the diagonal, zero otherwise), would be given by

$$\hat{I} = \sum_n |n\rangle\langle n| \tag{47}$$

Let us now define the matrix for the lowering operator:

$$\hat{a}|\Psi\rangle = \hat{a}\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ ...\end{pmatrix} = \textstyle\sum_{n=0}\psi_n\hat{a}|n\rangle = \sum_{n=0}\sqrt{n+1}\psi_{n+1}|n\rangle = \begin{pmatrix}\sqrt{1}\psi_1\\ \sqrt{2}\psi_2\\ \sqrt{3}\psi_3\\ ...\end{pmatrix}$$

We can achieve the same effect of applying an operator $\hat{a}$ to a general quantum state $|\Psi\rangle$ by using the following matrix multiplication:

$$\hat{a}|\Psi\rangle = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & ... \\ 0 & 0 & \sqrt{2} & 0 & ... \\ 0 & 0 & 0 & \sqrt{3} & ... \\ 0 & 0 & 0 & 0 & ... \\ ... & & & & \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \\ ... \end{pmatrix}$$

The raising operator matrix is obtained by a simple transposition:

$$\hat{a}^\dagger|\Psi\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 & ... \\ \sqrt{1} & 0 & 0 & 0 & ... \\ 0 & \sqrt{2} & 0 & 0 & ... \\ 0 & 0 & \sqrt{3} & 0 & ... \\ ... & & & & \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \\ ... \end{pmatrix}$$

Exercise 23: Write down matrices for $\hat{x}$ and $\hat{p}$ operators using for $N_{max} = 4$. Do they come out hermitian?

Exercise 24: Write down matrices for $\hat{a}^\dagger a$ and $\hat{a}\hat{a}^\dagger$ operators for $N_{max} = 4$. Are these matrices identical?

Exercise 25: Use $N_{max} = 4$ and check if the commutation $[\hat{a}, \hat{a}^\dagger] = \hat{I}$, where $\hat{I}$ is the identity matrix. If it does not exactly match, how do you think we can fix it

We do not list here the matrix for $\hat{D}(\alpha)$ in the Fock basis, but this is an extremely useful matrix to have for all sorts of numerical calculations in quantum mechanics. In fact, designing a computationally efficient algorithm to generate the matrix for $\hat{D}$ in the Fock basis is an excellent course project!

E. Wavefunctions

So far we figured out the answer to the question "What is your energy?" for an oscillator in any state $|\Psi\rangle$. What if we instead want to ask a simingly simpler question "Where are you?". That is, we want to know the value of position x. Since $\hat{x} = x_0(\hat{a} + \hat{a}^\dagger)$ is a hermitian operator, quantum mechanics does allow asking such a question. Specifically, a hermitian operator $\hat{x}$ has real eigenvalues and eigenvectors, such that

$$\hat{x}|x = x'\rangle = x'|x = x'\rangle \tag{48}$$

A ket $|x = x'\rangle$ is an eigenvector of $\hat{x}$ with an eigenvalue x'. Just like the Fock states $|n\rangle, n = 0, 1, 2, ...)$ form an orthonormal basis, the eigenstates of $\hat{x}$ form a different orthonormal basis. We can expand a Fock state $|n\rangle$ in the basis of states $|x = x'\rangle$:

$$|n\rangle = \sum_{x'} \Psi_n(x')|x = x'\rangle \tag{49}$$

Likewise, we can expand a position eigenstate $|x\rangle$ over the energy eigenstates $|n\rangle$:

$$|x = x'\rangle = \sum_n \Psi_n^*(x')|n\rangle \tag{50}$$

The two decompositions are analogous to decomposing a $\hat{Z}$-eigenstate of a qubit in the $\hat{X}$-eigenstates basis and vice versa, except here the number of eigenstates in both basis is infinite. The amplitudes $\Psi_n(x)$ provide a (generally) complex number for each value of n and x. Just like in the case of qubits, we rely on the follwing orthogonality conditions:

$\langle n|n'\rangle = 0$
$\langle n|n\rangle = 1$
$\langle x = x'|x = x''\rangle = 0$
$\langle x = x'|x = x'\rangle = 1.$

Quantum measurement rule for the position observable. Now enters a delicate point. If the eigenvalues x' are discrete, just like the energy eigenvalues E_n, the probability that an oscillator in a Fock state $|n\rangle$ is found by a position measurement apparatus at a position $x = x'$ equals $|\Psi_n(x')|^2$. In that case we must use the normalization condition $\sum_{x'} |\Psi_n(x')|^2 = 1$. However, the eigenvalues of $\hat{x}$ are not discrete! Therefore, a question "What is your position" does not make sense (even classically). Instead, we have to ask "Are you between points $x = x'$ and $x = x' + \Delta x'$?", where $\Delta x'$ is some small position interval. For example, when you are using a ruler to measure the length of something, you are really deciding that the length is between the two closest gratings on the ruler. Therefore, we must slightly modify our quantum measurement rules for measuring a continuous observable $\hat{x}$. Namely, for an oscillator in a Fock state $|n\rangle$, the probability to measure the value of $\hat{x}$ between x' and $x' + dx'$ is given by

$$\mathrm{Prob(x' < x \leq x' + dx') = |\Psi_n(x')|^2 dx' \quad \Longrightarrow \int_{x=-\infty}^{x=+\infty} |\Psi_n(x)|^2 dx = 1} \tag{51}$$

In such a continuous limit the amplitude $\Psi_n(x)$ in the decomposition of a Fock state $|n\rangle$ over position eigenstates becomes a continuous function of position x. The function $\Psi_n(x)$ then called the "wavefunction" of state $|n\rangle$ and it contains all the information on this state.

Recursion relation for Fock-states wavefunctions. We know how $\hat{x}$ acts both on the energy eigenstates and on the position eigenstates:

$$\hat{x}|n\rangle = x_0\sqrt{n}|n-1\rangle + x_0\sqrt{n+1}|n+1\rangle = x_0 \sum_{x'} \Big(\sqrt{n}\Psi_{n-1}(x') + \sqrt{n+1}\Psi_{n+1}(x')\Big)|x = x'\rangle$$

$$\hat{x}|n\rangle = \sum_{x'} \Psi_n(x')\hat{x}|x = x'\rangle = \sum_{x'} x'\Psi_n(x')|x = x'\rangle$$

Comparing the two above expressions, we find the following recursive relation for $\Psi_n(x)$:

$$\Psi_{n+1}(x) = \frac{1}{\sqrt{n+1}}\Big(\frac{x}{x_0}\Psi_n(x) - \sqrt{n}\Psi_{n-1}(x)\Big) \tag{52}$$

with an implied condition $\Psi_{-1}(x) = 0$. All that is left to do is to find $\Psi_0(x)$, the wave-function corresponding to the oscillator's ground state. Then we can recursively generate all the excited-state wave-functions.

Exercise 26: Use the recursion relation in Eq. 52 to derive the following wave-functions

of the oscillator's excited state:

$$\Psi_1(x) = (x/x_0)\Psi_0(x) \tag{53}$$

$$\Psi_2(x) = \frac{1}{\sqrt{2}}\Big[(x/x_0)^2 - 1\Big]\Psi_0(x) \tag{54}$$

$$\Psi_3(x) = \frac{1}{\sqrt{6}}(x/x_0)\Big[(x/x_0)^2 - 3\Big]\Psi_0(x) \tag{55}$$

$$... \tag{56}$$

QuTiP has these already coded so it is easy to plot them and see where a quantum oscillator is in various states. But first we need to somehow find $\Psi_0(x)$! For that we have to study the momentum operator.

Momentum operator in the position eigenstates basis. We already had a hint that momentum operator generates displacements along x. So we take a displacement operator and use its commutations properties from (Eq. 46). Choosing a small position change δx and $\alpha = \delta x/2x_0$ and applying the commutation relation in Eq. 46, we get

$$\exp\Big(-\frac{i\hat{p}\delta x}{\hbar}\Big)|x = x'\rangle = |x = x' + \delta x\rangle \tag{57}$$

Assuming δx is sufficiently small, we Taylor-expand the matrix exponent to the first order:

$$\exp(-i\hat{p}\delta x/\hbar) \approx 1 - i\hat{p}\delta x/\hbar \tag{58}$$

from which we conclude that

$$\hat{p}|x = x'\rangle = (+i\hbar)\frac{|x = x' + \delta x\rangle - |x = x'\rangle}{\delta x} \tag{59}$$

Next, apply $\hat{p}$ to an arbitrary state Fock state:

$$\hat{p}\sum_x \Psi_n(x)|x\rangle = \frac{i\hbar}{\delta x}\sum_x \Psi_n(x)|x + \delta x\rangle - \Psi_n(x)|x\rangle = \frac{i\hbar}{\delta x}\sum_x \Psi_n(x - \delta x)|x\rangle - \Psi_n(x)|x\rangle$$

Taking the limit $\delta x \to 0$, we get

$$\hat{p}\sum_x \Psi_n(x)|x\rangle = \sum_x (-i\hbar)\frac{\partial\Psi_n(x)}{\partial x}|x\rangle \tag{60}$$

Thus, acting with the operator $\hat{p}$ on a Fock state ket $|n\rangle$, expanded **in the position eigenstates basis**, is equivalent to replacing the corresponding wavefunction $\Psi_n(x)$ according to the following rule: $\Psi_n(x) \to -i\hbar\partial\Psi_n(x)/\partial x$. This property of momentum operators allows us to find a differential equation for the ground state wave-function:

$$\hat{a}|0\rangle = \Big[\frac{\hat{x}}{2\hat{x}_0} + \frac{i\hat{p}}{2p_0}\Big]|0\rangle = \sum_x \Psi_0(x)\Big[\frac{\hat{x}}{2\hat{x}_0} + \frac{i\hat{p}}{2p_0}\Big]|x\rangle = \sum_x \Big[\frac{x\Psi_0(x)}{2x_0} + x_0\frac{\partial\Psi_0(x)}{\partial x}\Big]|x\rangle \tag{61}$$

Since the expression above must equal to the null-vector, we have to set all amplitudes in front of each $|x\rangle$ to zero, which yields

$$x\Psi_0(x) + 2x_0^2\frac{\partial\Psi_0(x)}{\partial x} = 0 \tag{62}$$

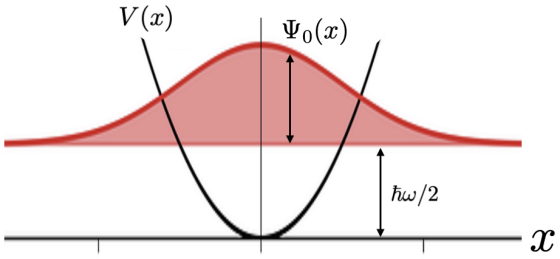

Figure 4: Combined plot of the harmonic oscillator potential $V(x)$ and the ground state wavefunction $\Psi_0(x)$ (measured from the horizontal thin line, which in tern defines the ground state energy level $\hbar\omega/2$.)

Exercise 27: Verify that the following function satisfies Eq. 62:

$$\Psi_0(x) = \frac{1}{(2\pi x_0^2)^{1/4}} \exp\Big[-(x/2x_0)^2\Big] \tag{63}$$

Exercise 28: Plot the 3 lowest energy eigenstates wavefunctions using the same X-axis (stack the plots vertically). Count the number of nodes (zero-value crossing). Make a similar plot with $|\Psi|^2$. Are you surprised with where the oscillator is more or less likely to be?

Exercise 29: Verify by numerical integration that $\Psi_0(x)$, $\Psi_1(x)$, and $\Psi_2(x)$ magically come out normalized in the sense of Eq. 51.

Exercise 30: Verify by numerical integration that $\Psi_0(x)$, $\Psi_1(x)$, and $\Psi_2(x)$ magically come out orthogonal, that is

$$\int_{-\infty}^{+\infty} \Psi_0(x)\Psi_1(x)dx = \int_{-\infty}^{+\infty} \Psi_1(x)\Psi_2(x)dx = \int_{-\infty}^{+\infty} \Psi_2(x)\Psi_0(x)dx = 0 \tag{64}$$

Circling back to the query "where are you?", we can now calculate the probability that the oscillator in a Fock state $|n\rangle$ is located between position values x_1 and x_2:

$$\mathrm{Prob}[\mathrm{x_1} \le \mathrm{x} \le \mathrm{x_2}] = \int_{\mathrm{x_1}}^{\mathrm{x_2}} |\Psi_\mathrm{n}(\mathrm{x})|^2 \mathrm{dx} \tag{65}$$

With a few exceptions, it's best to do such integrals numerically. We remind that the geometric meaning of an integral is the area underneath the function $|\Psi_n(x)|^2$, so even if one cannot do the integral accurately, one can still get an idea of the answer.

Exercise 31: Plot $|\Psi_n(x)|^2$ for $n = 0, 1, 2$. For each n, calculate the probability that $|x| < x_{\mathrm{RMS}}$, which we calculated in Exercise 2 (x_{RMS} varies with n).

F. Discovering quantum mechanics with oscillator wavefunctions.

Classically forbidden region. We have already seen that a quantum oscillator kind of can't stop moving in its ground state $|0\rangle$. With the instrument of wavefunctions we can

furthermore discover that a quantum oscillator can be found in places where a classical one is just not allowed to be! Indeed, since the kinetic energy cannot be negative, a classical oscillator with energy E must stop whenever $V(x) = m\omega^2 x^2/2 = E$ (because then $p^2/2m = 0$). Therefore, a classical oscillator with energy E can never be found at a position x satisfying $|x| > x_c = \sqrt{2E/m\omega^2}$. Is this the case for a quantum oscillator?

Suggestion for numerical analysis. We recommend defining a harmonic oscillator via two parameters: the frequency ω and x_0 which by now you know is related to the size of the quantum fluctuations of x. It would also be helpful to always normalize position by x_0 and energy by $\hbar\omega$ in your plots.

Exercise 32: Plot the oscillator's potential energy $V(x) = m\omega^2 x^2/2 = \hbar\omega(x^2/4x_0^2)$ and identify the classically forbidden region geometrically for the ground state $\Psi_0(x)$.

Exercise 33: Stack the plot from the precious exercise on top of a plot for $|\Psi_0(x)|^2$, using exactly the same range of x-axis. We call it the "$V(x) - \Psi(x)$" plot. Observe that there is a non-zero probability to find the oscillator at $|x| > x_c$. Indicate this probability geometrically (corresponding area underneath the probability density function).

Exercise 34: Make the "$V(x) - \Psi(x)$" plot for $|\Psi_{100}|^2$ and observe that one is more likely to find a paticle near the boundaries of the classically forbidden region. Does this make sense with your classical intuition?

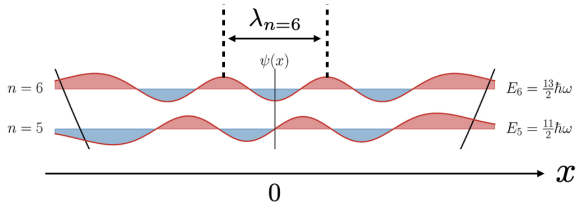

Figure 5: Illustration of the De Broglie wavelength notion using state $|n = 6\rangle$. Near $x = 0$ we can neglect the potential energy and hence we seeing a wave-function of a nearly free particle with a momentum equal to $|p| = \sqrt{2mE_6}$.

De Broglie wavelength. Consider the wavefunction $\Psi_{10}(x)$ Observe how the wavefunction (and hence the probability density) oscillates in x. Let's zoom in on a couple of periods near $x = 0$. In that region $V(x) \ll E$, so the potential energy may be neglected, and we can equate $E \approx p^2/2m$. This gives us the value of momentum in state $\Psi_{10}(x)$ near $x = 0$, $p \approx \sqrt{2mE_{10}}$. We can convert this value of momentum into a length scale using a relation

$$\lambda = 2\pi\hbar/p \tag{66}$$

The length scale λ is called De Broglie wavelength. Thus, the Plank's constant not only converts frequency to energy but it also converts wavelength to momentum. Every particle with a momentum p is associate with a wave in real space, the wavelength of which is given by the De Broglie wavelength. This is a probability wave, it shows that the probability to find a particle in a given small interval of positions oscillates in space. It is in that sense a quantum particle can behave as a wave. The heavier the particle and the larger its energy, the smaller the wavelength and hence the harder it is to resolve the oscillations.

Exercise 34: Calculate De Broglie wavelength of a cat chasing a mouse. Use any realistic assumptions on the mass and the speed of the cat.

Exercise 35: Plot $\Psi_{10}(x)$, zoom in to its period near the center $x = 0$, and extract the period (which would have the units of length). Verify that this period indeed approximately equals to $2\pi x_0/\sqrt{10 + 1/2}$ for the Fock state $|10\rangle$.

Exercise 36: Repeat the previous exercise and identify the De Broglie wavelength λ_n for states $|n\rangle$, $n = 10, 20, 30, .., 100$. Summarize your answers on a λ_n vs n plot and compare them to the analytical prediction $\lambda_n = 2\pi x_0/\sqrt{n}$.

Evolution of a state with "better known" position. Let's see just how much a quantum oscillator does not want to have an exact position. Let us prepare a comparatively well-localized state

$$|\Phi\rangle = \sum_{x'} \Phi(x')|x = x'\rangle, \quad \Phi(x) = \exp(-(x/2a)^2) \tag{67}$$

By choosing $a < x_0$, we make $|\Phi\rangle$ not an energy eigenstate, so it must evolve in time. How to work out this evolution? The same ket can be decomposed over the Fock states:

$$|\Phi\rangle = \sum_n \phi_n |n\rangle \tag{68}$$

Therefore,

$$\Phi(x) = \langle x|\Phi\rangle = \sum_n \phi_n \Psi_n(x) \tag{69}$$

Important: the two above equations allow us to find a wavefunction $\Phi(x)$ associated with any ket vector $|\Phi\rangle$ as soon as we find out the amplitudes ϕ_n for its decomposition over the Fock states. **Very useful trick!** Here we are solving the reverse problem, we already know $\Phi(x)$ and we want to find the amplitudes ϕ_n. To do that we use the orthogonality properties of position and energy eigenstates::

$$\sum_x \Phi(x)\Psi_m(x) = \sum_n \phi_n \sum_x \Psi_n(x)\Psi_m(x) \tag{70}$$

Recalling that x is a continuous variable, we must replace the summation with integration:

$$\sum_x \Psi_n(x)\Psi_m(x) \to \int_{x=-\infty}^{x=+\infty} \Psi_n(x)\Psi_m(x)dx = \delta_{n,m} \tag{71}$$

$$\sum_x \Phi(x)\Psi_n(x) \to \int_{x=-\infty}^{x=+\infty} \Phi(x)\Psi_n(x)dx = \phi_n \tag{72}$$

$$\tag{73}$$

And the time evolution of $|\Phi(t)\rangle$ is given by

$$|\Phi(t)\rangle = \sum_n \phi_n \exp(-in\omega t)|n\rangle \tag{74}$$

$$\phi_n = \int_{x=-\infty}^{x=+\infty} \Phi(x)\Psi_n(x)dx \tag{75}$$

$$\Phi(x,t) = \sum_n \phi_n \exp(-in\omega t)\Psi_n(x) \tag{76}$$

Eq. 76 defines the evolution of an arbitrary initial quantum state in both time and space.

Exercise 37: Make a movie for a time-evolution in Eq. 76 using the initial state $\Phi(x) = \exp(-(x/2a)^2)$ and try $a = x_0$ (nothing should evolve), $a = x_0/2$, $a = x_0/10$, $a = x_0/100$. To implement the numerics, use $N_{max} = 50$ and plot $|\Phi(x,t)|^2$. Experiment with the time step and the total time duration to make sure you don't miss any action.

Evolution of a coherent state. Eq. 76 describes in fact the time-evolution starting from an arbitrary state. Let's apply it to a couple of more familiar initial states.

Exercise 38: Make a movie for a time-evolution in Eq. 76 starting from a coherent state α defined in Eq. 28. In this case we already know that $\phi_n = (\alpha)^n/\sqrt{n!}$ (up to a constant). Try $\alpha = 1, 2, 10$. Do you imagine classical oscillator moving that way?

Exercise 39: Make a movie for a time-evolution in Eq. 76 starting from a state $\frac{1}{\sqrt{2}}|n=0\rangle + \frac{1}{\sqrt{2}}|n=10\rangle$. Do you imagine classical oscillator moving that way? Take a few of your favorite snapshots for the homework report.

G. Quantum mechanics beyond harmonic oscillator (extra credit)

Weakly anharmonic oscillator. By now we have built up tools to study main aspects of quantum-mechanical bound motion, not just restricted to harmonic oscillators. The Python implementation of these exercises will be discussed in the seminars.

Exercise 40: Consider a system with a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$, where $\hat{H}_0 = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2)$ is the standard harmonic oscillator Hamiltonian and there is an additional energy term $\hat{H}_1 = \hbar K(a + a^\dagger)^4$ where $K = \omega/10$. This term would come up in the case of an anharmonic potential energy $V(x) = m\omega^2x^2/2 + K(x/x_0^4)$, think of a spring that stiffens as it is stretched more. **Question:** find numerically the 4 lowest energy eigenvalues and eigenstates of $\hat{H}$ using the energy eigenstates of $\hat{H}_0$.

Hint: For example, we can choose $N_{max} = 50$, define the matrices $\hat{a}$ and $\hat{a}^\dagger$, and build the full Hamiltonian matrix using the matrix multiplication. And proceed with an eigensolver.

Comment: For $K = 0$ we get $H = H_0$ so the Hamiltonian matrix should come out diagonal with familiar oscillator eigenvalues. Once you add $K \neq 0$, the energy eigenavlues will change, and the eigenstates would be superpositions of Fock states:

$$|E_k\rangle = \sum_{n=0}^{n=N_{max}} \phi_n(k)|n\rangle$$

The eigensolver will spit out N_{max} values of E_k and corresponding lists of $\phi_n(k)$ for each k. Usually this approach captures well the lowest energy eigenstates. The more eigenstates we would like to capture accurately, the higher the value of N_{max} we must choose. The way to verify you have chosen a good value N_{max} for the task is to double it and observe that the the eigenvalues change negligibly

Exercise 41: Obtain the wavefunction for the lowest four energy states $\Phi_0(x)$, $\Phi_1(x)$, $\Phi_2(x)$, and $\Phi_3(x)$ which are given by Eq. 69. For example:

$$\Phi_0(x) = \sum_{n=0}^{n=N_{max}} \phi_n(k=0)\Psi_n(x) \tag{77}$$

where $\Psi_n(x)$ are the familiar Fock states wavefunctions and the amplitudes ϕ_n for each $k = 0, 1, 2, 2$ are the components of your eigenvectors in the previous exercise. Plot $\Phi_0(x)$ against $\Psi_0(x)$, etc., and observe the changes in the wavefunction that the K-term brings.

From a weakly anharmonic oscillator to a qubit. Let us apply an external drive signal at a frequency ω_d to our weakly anharmonic oscillator, at a frequency close to $\omega == (E_1 - E_0)/\hbar$. Such a drive corresponds to a new term in the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + (\hat{a} + \hat{a}^\dagger) g \cos\omega_d t \tag{78}$$

To setup the time-dependent Schrodinger's equation, it's best to use the basis of eigenstates of $\hat{H}_0 + \hat{H}_1$, obtained for some N_{max} and truncate it to a small number M_{max} of the lowest energy states (we start in the ground state and we do not expect to go far...). In the basis of eigenstates of $\hat{H}_0 + \hat{H}_1$, the matrix for $\hat{H}_0 + \hat{H}_1$ is already diagonal. All we need is to calculate the the matrix $(\hat{a} + \hat{a}^\dagger)$ in this new basis and arrive at a $M_{max} \times M_{\max}$ matrix for the time-dependent Hamiltonian. Then we duly solve the time-dependent Schrodinger's equation and plot the probabilities of finding the system in any of the M_{max} eigenstates of the un-driven Hamiltonian. This method is in direct analogy with the Rabi oscillations problem for a qubit.

Exercise 42: Define states $|0\rangle$, $|1\rangle$, $|2\rangle$ as the three lowest energy eigenstates of $\hat{H}_0 + \hat{H}_1$. Set $K = \omega/10$. The corresponding eigenenergies are E_0, E_1, E_2. Introduce the drive term at a frequency $\omega_d = (E_1 - E_0)/\hbar$ and set $g = \omega/100$ and solve for the resulting time-dependent wave-function. Plot the probabilities of finding the system in states $|0\rangle$, $|1\rangle$, and $|2\rangle$ as a function of time on the same plot.

N.B. If the probability to find the system in state $|2\rangle$ is nearly zero, then it's as if there is no state $|2\rangle$. So, as long as we drive an anharmonic oscillator not too strongly and not far from the resonance, only the two resonating states matter, and the system behaves as a qubit!

Exercise 43: Repeat the previous exercise for a stronger drive amplitude $g = \omega/50$, $g = \omega/25$, $g = \omega/10$. See if you notice effects of populating state $|2\rangle$. In this case your system does not qualify to be a qubit.

Quantum tunneling through the energy barrier. Let us consider yet another deviation from a Harmonic oscillator, a system described by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$, where this time $\hat{H}_1 = B\cos\left[2\pi(\hat{x}/x_0)\right]$, and H_0 is the original Harmonic oscillator Hamiltonian. Let us further consider the value of B such that $B = 10 \times \hbar\omega$. Classically this Hamiltonian describes the motion of a particle in a "double-well" potential given by $V(x) = (\hbar\omega/4)(x/x_0)^2 + B\cos(2\pi x/x_0)$. Such a potential has two local minima positioned approximately at $x = \pm x_0$. A particle with an energy less than $2B$ will have to be stuck oscillating in one or the other well, but it cannot relocate from one to another. Is

this so in quantum mechanics?

We can solve for the spectrum and the wavefunctions of the lowest energy states in complete analogy with previous problems. All we need to do is to work out the matrix for $\hat{H}_1$ in the basis of the eigenstates of $\hat{H}_0$. We note that this Hamiltonian can be expressed via the good-old displacement operators:

$$H_1 = \frac{B}{2}\Big(\hat{D}(2\pi i) + \hat{D}^\dagger(-2\pi i)\Big) \tag{79}$$

There are various ways to create the matrix, it's quite an exercise on its own, but fortunately it's been done in most known numerical packages.

Exercise 44: Calculate the lowest 10 eigenenergies and eigenvectors (along with their wavefunctions) and analyze the results. Observe that the energy difference between the lowest two energy states is much smaller than to the second excited state. Also observe that despite the energy of the lowest two states is far below the top of the barrier, the wavefunction is non-zero in both local minima at the same time. Somehow, the particle "tunnels" through the barrier. This phenomenon is called quantum tunneling. It's related to the fact that a quantum particle can be in the classically forbidden zone, albeit with a suppressed probability.

Exercise 45: Consider any state localized in the left well as the initial condition for the Hamiltonian $\hat{H}_0 + \hat{H}_1$ in the previous problems. Calculate the time-evolution of this wavefunction and make a movie of the probability density. Observe how a particle oscillates between being in the left well and in the right well, being in both wells at the same at the half-time. How crazy is that? But that's an excellent way to make a qubit, because the second excited state is far-far off-resonance.

H. Wavefunctions of position and momentum eigenstates in a truncated Fock-basis (extra credit)

Here I invite you to play with numerically calculated eigenvalues of $\hat{x}$ and $\hat{p}$ using a basis of N_{max} lowest energy eigenstates, and examine the wavefunctions of the resulting ket's. Indeed, what is a wavefunction $\Psi_{x'}(x)$ for a position eigenstate $|x = x'\rangle$? On one hand, the very definition of it says it must be zero everywhere apart from $x = x'$. And it needs to be normalized. So the answer should be $\Psi_x(x) = \delta(x)$, something known in calculus as the delta-function. On the other hand, we can construct a matrix $\hat{x} = x0(\hat{a} + \hat{a}^\dagger)$ for a given N_{max} in the Fock basis, duly find its eigenvalues and eigenvectors, and use the construction in Eq. 69. We will find that the answer surely depends on N_{max} and in the limit $N_{max} \to \infty$ we would indeed find that for every eigenvalue x', we get $\Psi_{x'}(x) = \delta(x - x')$. In other words, to define a position eigenstate rigorously we need an infinite number of energy eigenstates! This sounds especially crazy if we just want to prepare an oscillator at rest at a position $x = 0$: – yet, in this state, no matter how high oscillator energy you choose (number of quanta, to be precise), there is a non-zero probability for this to happen. Let's make sense of this by considering the approximate wavefunctions of position eigenstates while increasing the number N_{max}

Exercise 46: Choose a value of $N_{max} = 10$ and calculate the eigenvalues of $\hat{x}$ matrix in the Fock basis. Choose an eigenvalue x closest to 0 and use the corresponding eigenvector

$$\begin{pmatrix} \psi_{x=0,0} \\ \psi_{x=0,1} \\ \psi_{x=0,2} \\ \dots \\ \psi_{x=0,N_{max}} \end{pmatrix}$$

to construct the wavefunction according to Eq. 69: $\Psi_{x=0}(x) = \sum_{n=0}^{n=N_{max}} \psi_{x=0,n}\Psi_n(x)$. Try $N_{max} = 10, 20, 100$. Normalize the X-axis by x_0. Try various eigenvalues of x.

Exercise 47: Replace the matrix for $\hat{x}$ with the matrix for $\hat{p}$ and repeat the previous exercise. The resulting wave-function would now describe momentum eigenstates in the truncated Fock basis. What do we know about those wavefunctions? Well, they should correspond to the De Broglie waves, with a wavelength linked to the chosen momentum eigenvalue. Check if this works. Start with the lowest absolute values of p (longer De Broglie wavelength).

I. Algebraic derivation of $\Psi_0(x)$ (extra credit)

In what follows, we are going to present a rather unusual but elegant method for finding $\Psi_0(x)$ using properties of displacement operators applied to ground state and to position eigenstates.
First, we recall that for any value of the position x' we have (see Eq. 48)

$$\Psi_0(x') = \langle x = x'|0\rangle \tag{80}$$

All we need is to find how this inner product depends on x'. The first trick is to move the dependence on x' from the state to an operator using Eq. 46:

$$|x = x'\rangle = \hat{D}(\alpha = x'/2x_0)|x = 0\rangle \implies \langle x = x'| = \langle x = 0|\hat{D}^\dagger(x'/2x_0) \tag{81}$$

Next, we develop the displacement operator $\hat{D}$ using the BCH formula (see Eq. 40):

$$\hat{D}^\dagger(x'/2x_0) = \exp\Big[\frac{-x'\hat{a}^\dagger + x'\hat{a}}{2x_0}\Big] = \exp\Big[-\frac{1}{2}(x'/2x_0)^2\Big]\exp\Big[-\frac{x'\hat{a}^\dagger}{2x_0}\Big]\exp\Big[\frac{x'\hat{a}}{2x_0}\Big] \tag{82}$$

Next, we take advantage of the ground state property (see Eq. 38) and shamelessly change the sign in front of $\hat{a}$ in the rightmost operator in Eq. 82 from + to -: :

$$\exp\Big[+\frac{x'\hat{a}}{2x_0}\Big]|0\rangle = \exp\Big[-\frac{x'\hat{a}}{2x_0}\Big]|0\rangle = |0\rangle \tag{83}$$

$$\hat{D}(x'/2x_0)|0\rangle = \exp\Big[-\frac{1}{2}(x'/2x_0)^2\Big]\exp\Big[-\frac{x'\hat{a}^\dagger}{2x_0}\Big]\exp\Big[-\frac{x'\hat{a}}{2x_0}\Big]|0\rangle \tag{84}$$

Next, we apply the BCH formula again and replace $\hat{a} + \hat{a}^\dagger = \hat{x}/x_0$:

$$\hat{D}(x'/2x_0)|0\rangle = \exp\Big[-\frac{1}{2}(x'/2x_0)^2\Big]\exp\Big[-\frac{1}{2}(x'/2x_0)^2\Big]\exp\Big[\frac{\hat{x}x'}{2x_0^2}\Big]|0\rangle \tag{85}$$

Finally, it is time to take advantage of

$$\langle x = 0|\exp\Big[\frac{\hat{x}x'}{2x_0^2}\Big] = \langle x = 0| \tag{86}$$

to arrive at

$$\Psi_0(x) = \exp\Big[-(x/2x_0)^2\Big] \times \langle x = 0|0\rangle \tag{87}$$

The remaining overlap between the $x = 0$ position eigenstate and the ground state $\langle x = 0|0\rangle$ is merely a constant, which can be found from the normalization condition $\int_{-\infty}^{+\infty} |\Psi_0(x)|^2 dx = 1$. This is a Gaussian integral, so we can just look it up to arrive at the final-final answer for the ground-state wave function of a quantum harmonic oscillator:

$$\Psi_0(x) = \frac{1}{(2\pi x_0^2)^{1/2}} \exp\Big[-(x/2x_0)^2 \Big] \tag{88}$$

Exercise 48: You might have noticed by now that position and momentum enter quite symmetrically into the oscillator algebra. So, can you repeat the above analysis to find the wavefunction $\tilde{\Psi}_0(p)$ of the ground state $|0\rangle$ in the basis of **momentum eigenstates**? These momentum wavefunctions would allow us to know the distribution of momentum for a harmonic oscillator, that is how likely it is to have this momentum over that momentum in each energy eigenstate.