Physics 143a – Workshop 7

Quantum Mechanical Harmonic Oscillator

Week Summary

- **Raising and Lowering Operators:** When modeling harmonic oscillator systems it is useful to write the system's Hamiltonian in terms of raising and lowering operators. Namely, suppose we have a Hamiltonian given by

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{X}^2, \tag{1}$$

where $\hat{P}$ is the momentum operator, $\hat{X}$ is the position operator, m is the mass of the particle within the well, and ω is the well's angular frequency. We can then define the raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$ by

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{X} - \frac{i}{m\omega}\hat{P}\right), \qquad \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{X} + \frac{i}{m\omega}\hat{P}\right), \tag{2}$$

such that the Hamiltonian now becomes

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{3}$$

In deriving Eq.(3), we used the Heisenberg Uncertainty principle and Eq.(2), to establish and apply the identity

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{4}$$

Labeling the system's energy eigenkets as $|n\rangle$ (where $n = 0, 1, \ldots$), the action of the raising and lowering operators on the eigenkets is

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \qquad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{5}$$

Using Eq.(5) in Eq.(3), we find that the energy eigenvalues of the harmonic oscillator are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{6}$$

- **Wave Function Solutions:** The Time-Indepdent Schrödinger equation for the Harmonic Oscillator in the position basis is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi_n(x) = E_n\psi_n(x). \tag{7}$$

The energy eigenvalues are given by Eq.(6), and the eigenfunction solutions are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)e^{-m\omega x^2/2\hbar} \tag{8}$$

where $H_n(x)$ is a Hermite Polynomial given by (among other formulas) the generating function

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2/2}. \tag{9}$$

1 Problems

1. **Coherent (i.e., quasi-classical) states of the harmonic oscillator**
   Certain linear combinations of harmonic oscillator states (known as 'coherent states') satisfy $\Delta x \Delta p = \hbar/2$ and thus minimize the uncertainty limit. These states are also known as 'quasi-classical' because they have position and momentum expectation values which match the classical behavior of an oscillator.

   These coherent states are eigenfunctions of the lowering operator:

   $$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{10}$$

   where we take $|\alpha\rangle$ to be a normalized state and $\alpha \in \mathbb{C}$.

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

   $$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle. \tag{11}$$

   Using Eq.(10) determine the expansion coefficients c_n (for $n \geq 1$) in terms of c_0.

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

   (c) Say we have a state $|\psi(0)\rangle = |\alpha\rangle$ at time $t = 0$. Using the fact that an overall phase factor does not change the nature of the state, what is the state $|\psi(t)\rangle$? Write the result in terms of $|\alpha(t)\rangle \equiv |\alpha e^{-i\omega t}\rangle$. (*Hint:* You would need to remember how to transform a time-independent state into a time-dependent one.)

   (d) Say we have a classical harmonic oscillator with amplitude X_0, mass m, frequency ω, and phase ϕ. What are the classical oscillator's position and momentum as functions of time?

   (e) Compute $\langle\alpha(t)|\hat{X}|\alpha(t)\rangle$ and $\langle\alpha(t)|\hat{P}|\alpha(t)\rangle$ and simplify as much as possible. (*Hint:* Recall that $\hat{a}^\dagger$ is the hermitian conjugate of $\hat{a}$.)

   (f) What is the correspondence between the results in (d) and (e)?

2 Solutions

1. (a) Beginning from the expansion of the coherent state in terms of energy eigenstates and acting on it with the lowering operator, we find

$$\begin{aligned} \alpha|\alpha\rangle &= \hat{a}|\alpha\rangle \\ \sum_{n=0}^{\infty} c_n \alpha |n\rangle &= \sum_{n=0}^{\infty} c_n \hat{a}|n\rangle \\ \sum_{n'=1}^{\infty} c_{n'-1}\alpha|n'-1\rangle &= \sum_{n=0}^{\infty} c_n \sqrt{n}|n-1\rangle \\ &= \sum_{n=1}^{\infty} c_n \sqrt{n}|n-1\rangle, \end{aligned} \tag{12}$$

where we made the change of integration variables $n = n' - 1$ in the third line. From the final line, we can conclude that $c_n = \alpha c_{n-1}/\sqrt{n}$. Iterating this result gives us

$$c_n = \frac{\alpha c_{n-1}}{\sqrt{n}} = \frac{\alpha^2 c_{n-2}}{\sqrt{n(n-1)}} = \cdots = \frac{\alpha^n c_0}{\sqrt{n!}}, \tag{13}$$

which determines the coherent state up to an overall normalization c_0.

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(b) Requiring the previously found coherent state to be normalized, we have

$$\begin{aligned} 1 &= \langle\alpha|\alpha\rangle \\ &= \sum_{\ell,n=0}^{\infty} c_\ell^* c_n \langle \ell|n\rangle \\ &= \sum_{\ell,n=0}^{\infty} \frac{c_0^* \alpha^{*\,\ell}}{\sqrt{\ell!}} \frac{c_0 \alpha^n}{\sqrt{n!}} \langle \ell|n\rangle \\ &= \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!}|c_0|^2 \\ &= e^{|\alpha|^2}|c_0|^2. \end{aligned} \tag{14}$$

Thus we can infer that $c_0 = e^{-|\alpha|^2/2}$.

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(c) To find the time-dependent coherent state, we apply the time-evolution operator to the original coherent state:

$$\begin{aligned} e^{-i\hat{H}t/\hbar}|\alpha\rangle &= e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i\hat{H}t/\hbar}|n\rangle \\ &= e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega(n+1/2)t}|n\rangle \\ &= e^{-i\omega t/2}e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} \\ &= e^{-i\omega t/2}|\alpha e^{-i\omega t}\rangle. \end{aligned} \tag{15}$$

Given that the constant phase factor in Eq.(15) is not physically significant, we can conclude that time evolving the coherent state appends an exponential phase to the coherent state parameter α:

$$e^{-i\hat{H}t/\hbar}|\alpha\rangle \to |\alpha(t)\rangle, \tag{16}$$

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

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(d) For a classical oscillator with amplitude X_0, mass m, frequency ω, and phase ϕ, the position and momentum solutions to the equations of motion are

$$X(t) = X_0 \cos(\omega t + \phi), \quad P(t) = -m\omega X_0 \sin(\omega t + \phi). \tag{17}$$

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(e) The complex exponential form of $\alpha(t)$ is

$$\alpha(t) = \alpha e^{-i\omega t} = |\alpha| e^{-i\omega t + \phi_\alpha}, \tag{18}$$

where $\tan\phi_\alpha = \text{Im}(\alpha)/\text{Re}(\alpha)$. Thus, computing the expectation value of the position and momentum operators for a time-dependent coherent state, we find

$$\begin{aligned}\langle\alpha(t)|\hat{X}|\alpha(t)\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}^\dagger + \hat{a}|\alpha\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}(\alpha^*(t) + \alpha(t)) = |\alpha|\sqrt{\frac{2\hbar}{m\omega}}\cos(\omega t - \phi_\alpha), \end{aligned}\tag{19}$$

$$\begin{aligned}\langle\alpha(t)|\hat{P}|\alpha(t)\rangle &= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{i}\langle\alpha|\hat{a} - \hat{a}^\dagger|\alpha\rangle \\ &= \sqrt{\frac{\hbar m\omega}{2}}\frac{1}{i}(\alpha(t) - \alpha(t)^*) = -|\alpha|\sqrt{2\hbar m\omega}\sin(\omega t - \phi_\alpha). \end{aligned}\tag{20}$$

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(f) As is true to its name, the quasi-classical state $|\alpha(t)\rangle$ reproduces the time-dependent classical expectation values. Comparing the results of (d) and (e), we find the correspondence between the two results is given by

$$|\alpha|\sqrt{\frac{2\hbar}{m\omega}} \to X_0 \quad \text{and} \quad \phi_\alpha \to \phi. \tag{21}$$

Thus it is possible to go from coherent state expectation values to the corresponding physical results computed in the classical theory.

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30 min - Practice Exam

1. **(Stern-Gerlach Gravitino)**
   The gravitino, the hypothetical supersymmetric partner of the graviton (which is itself the hypothetical 'force carrier' of gravity), is a spin-3/2 fermion.

   Assume the gravitino has a magnetic moment which is proportional to its spin. We set up a Stern-Gerlach experiment where a beam of gravitinos is initially in a state where there is equal probability to be in any of its spin-$\hat{z}$ states. We then send the beam through a finite region containing a magnetic field pointing in the $\hat{z}$-direction. Draw a schematic of this experiment showing the beam before it enters and after it exits the field.

2. **(Photon Polarization)**
The matrix representation for a photon propagating along the z-axis of a quartz crystal (using the linear polarization states $|+\rangle$ and $|-\rangle$ as a basis) is given by

$$\hat{H} = \begin{pmatrix} 0 & -iE_0 \\ iE_0 & 0 \end{pmatrix}, \qquad \text{[In the } |+\rangle, |-\rangle \text{ basis].} \tag{22}$$

(a) What are the eigenstates (in the $|+\rangle, |-\rangle$ basis) and eigenvalues of the Hamiltonian?

(b) A photon enters the crystal in the state $|\psi(0)\rangle = |+\rangle$. What is the probability to find the photon in this initial state at time t?

3. **Lennard-Jones potential**

The potential energy of two atoms separated by a distance r is often well represented by the Lennard-Jones potential:

$$V(r) = \varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - 2 \left(\frac{\sigma}{r} \right)^{6} \right], \tag{23}$$

where ε and σ are parameters with the units of energy and length, respectively.

(a) Calculate the position r_0 of the potential energy minimum, and show (by determining V_0 and $m\omega^2$) that near $r = r_0$

$$V(r) \simeq \frac{1}{2} m\omega^2 (r - r_0)^2 + V_0. \tag{24}$$

(b) We have a quantum particle of mass m located near $r = r_0$. Write the energy eigenvalues of this system in terms of the parameters of Eq.(23).

4. **(Model of a diatomic molecule)**
Assuming $g > 0$, we can very crudely model the potential felt by an electron of a diatomic molecule as

$$V(x) = -\frac{\hbar^2 g}{2m}\Big[\delta(x+\ell) + \delta(x-\ell)\Big]. \tag{25}$$

The nuclear axis is taken to be the x axis, and the two nuclei are located at $x = +\ell$ and $x = -\ell$.

(a) For this potential, write the boundary conditions a solution of the Schrödinger equation must satisfy.

(b) Qualitatively sketch $|\psi(x)|^2$ (where $\psi(x)$ is a bound state wave function solution) and $V(x)$ labeling each plot and important positions along the x-axis.

3 Practice Exam Answers

1. Fig. 1

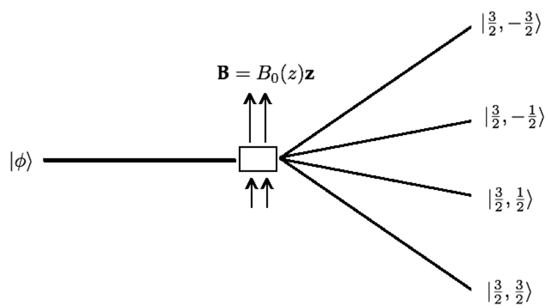

Figure 1: Stern-Gerlach for Gravitino: $|\phi\rangle = \frac{1}{2}|\frac{3}{2}, \frac{3}{2}\rangle + \frac{1}{2}|\frac{3}{2}, \frac{2}{2}\rangle + \frac{1}{2}|\frac{3}{2}, -\frac{1}{2}\rangle + \frac{1}{2}|\frac{3}{2}, -\frac{3}{2}\rangle$. Plot assumes the gravitino magnetic moment is the negative of the spin, and thus negative spins are pushed in the direction of increasing field. Actually, modern theories of the gravitino do not predict it to have a magnetic moment, although some models do have it interacting with the electromagnetic field.

2. (a)

$$|E_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad E_1 = E_0 \tag{26}$$

$$|E_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad E_1 = -E_0 \tag{27}$$

(b)

$$\text{Prob}(+ \to + \text{ transition in time } t) = |\langle +|\psi(t)\rangle|^2 = \cos^2(E_0 t/\hbar). \tag{28}$$

3. We find $r_0 = \sigma$ is the point where the potential is at a local minimum. The potential can then be written as

(a)

$$V(r) \simeq \frac{36\varepsilon}{\sigma^2}(r-\sigma)^2 - \varepsilon. \tag{29}$$

(b)

$$E_n = \hbar\sqrt{\frac{72\varepsilon}{m\sigma^2}}\left(n + \frac{1}{2}\right) \tag{30}$$

4. (a) The wave function must satisfy continuity across all potential boundaries and discontinuities in its derivative as defined by the potential.

$$\lim_{x\to\ell^+}\psi(x) = \lim_{x\to\ell^-}\psi(x), \qquad \left(\frac{d\psi(x)}{dx}\right)_{\ell^+} - \left(\frac{d\psi(x)}{dx}\right)_{\ell^-} = -g\psi(\ell) \tag{31}$$

$$\lim_{x\to-\ell^+}\psi(x) = \lim_{x\to-\ell^-}\psi(x), \qquad \left(\frac{d\psi(x)}{dx}\right)_{-\ell^+} - \left(\frac{d\psi(x)}{dx}\right)_{-\ell^-} = -g\psi(-\ell). \tag{32}$$

If we include the additional requirement that the particle is a bound state then we require $\psi(x) \to 0$ as $x \to \pm\infty$.

(b) Fig. 2

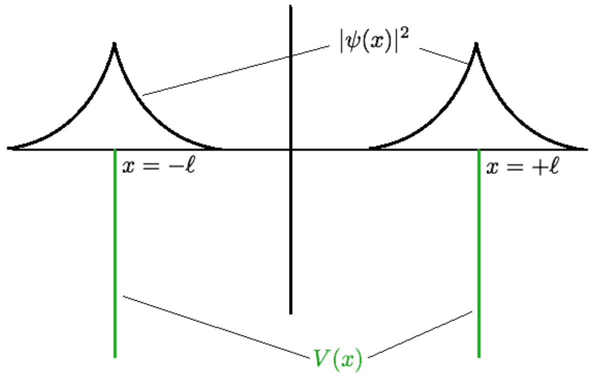

Figure 2: Potential and wave function magnitude: The potential is shown in green and the wave-function modulus squared is in black.