Lecture #9: Harmonic Oscillator: Creation and Annihilation Operators

Last time

Simplified Schrödinger equation: $\xi = \alpha^{1/2}x,\ \alpha = (k\mu)^{1/2}/\hbar$

$$\left[-\frac{\partial^2}{\partial\xi^2} + \xi^2 - \frac{2E}{\hbar\omega}\right]\psi = 0 \qquad \text{(dimensionless)}$$

reduced to Hermite differential equation by factoring out asymptotic form of ψ. The asymptotic ψ is valid as $\xi^2 \to \infty$. The exact ψ_v is

$$\psi_v(x) = N_v \underbrace{H_v}_{\text{Hermite polynomials}}(\xi)e^{-\xi^2/2} \qquad v = 0, 1, 2, \ldots \infty$$

orthonormal set of basis functions
$E_v = \hbar\omega(v + ½),\ v = 0, 1, 2, \ldots$
even v, even function
odd v, odd function
v = # of internal nodes
what do you expect about $\langle\hat{T}\rangle$? $\langle\hat{V}\rangle$? (from classical mechanics)
pictures

- * zero-point energy
- * tails in non-classical regions
- * nodes more closely spaced near $x = 0$ where classical velocity is largest
- * envelope (what is this? maxima of all oscillations)
- * semiclassical: good for pictures, insight, estimates of $\int \psi_v^* \hat{O}p\psi_{v'}$ integrals without solving Schrödinger equation

  $$p_E(x) = p_{\text{classical}}(x) = \left[2\mu\left(E - V(x)\right)\right]^{1/2}$$

  envelope of $\psi(x)$ in classical region (classical mechanics)

  $$\left(\psi^*\psi dx \propto \frac{1}{\underbrace{v}_{\text{velocity}}},\ \left|\psi(x)\right|_{\text{envelope}} = 2^{1/2}\left[\frac{2k/\pi^2}{E - V(x)}\right]^{1/4} \text{ for H. O.}\right)$$

  spacing of nodes (quantum mechanics): # nodes between x_1 and x_2 is

  $$\frac{2}{h}\int_{x_1}^{x_2} p_E(x)\,dx \quad \text{(because } \lambda(x) = h/p(x) \text{ and node spacing is } \lambda/2)$$

  \# of levels below E: $\frac{2}{h}\int_{x_-(E)}^{x_+(E)} p_E(x)\,dx$ "Semi-classical quantization rule"

  "Action (h) integral."

Non-Lecture

Intensities of Vibrational fundamentals and overtones from

$$\mu(x) = \mu_0 + \mu_1 x + \frac{1}{2}\mu_2 x^2 + \ldots$$

$$\int dx\ \psi_v^* x^n \psi_{v+m} \qquad \text{“selection rules”}$$

$$m = n, n-2, \ldots -n$$

Today some amazing results from $\widehat{\mathbf{a}^{\dagger}}, \hat{\mathbf{a}}$ (creation and annihilation operators)

* dimensionless $\hat{\tilde{x}}, \hat{\tilde{p}}$ $\rightarrow$ exploit universal aspects of problem — *separate universal from specific* $\rightarrow$ $\hat{\mathbf{a}}, \hat{\mathbf{a}}^{\dagger}$ annihilation/creation or “ladder” or “step-up” operators
* integral- and wavefunction-free Quantum Mechanics
* all E_v and ψ_v for Harmonic Oscillator using $\hat{\mathbf{a}}, \hat{\mathbf{a}}^{\dagger}$
* values of integrals involving all integer powers of $\hat{x}$ and/or $\hat{p}$
* “selection rules”
* integrals evaluated on sight rather than by using integral tables.

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1. Create dimensionless $\hat{\tilde{x}}$ and $\hat{\tilde{p}}$ operators from $\hat{x}$ and $\hat{p}$

$$\hat{x} = \left[\frac{\hbar}{\mu\omega}\right]^{1/2} \hat{\tilde{x}}, \qquad \text{units } = \left[\frac{m\ell^2 t^{-1}}{mt^{-1}}\right]^{1/2} = \ell \qquad \left(\text{recall } \xi = \alpha^{1/2} x = \left[\frac{k\mu}{\hbar^2}\right]^{1/4} x\right)$$

$$\hat{p} = [\hbar\mu\omega]^{1/2}\, \hat{\tilde{p}}, \qquad \text{units } = \left[m\ell^2 t^{-1} m t^{-1}\right]^{1/2} = m\ell t^{-1} = p$$

replace $\hat{x}$ and $\hat{p}$ by dimensionless operators

$$\widehat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}k\hat{x}^2 = \underbrace{\frac{\hbar\mu\omega}{2\mu}}_{\frac{\hbar\omega}{2}}\hat{\tilde{p}}^2 + \underbrace{\frac{k}{2}\frac{\hbar}{m\omega}}_{\frac{\hbar\omega}{2}}\hat{\tilde{x}}^2$$

$$= \frac{\hbar\omega}{2}\left[\hat{\tilde{p}}^2 + \hat{\tilde{x}}^2\right] \qquad \text{factor this?}$$

$$= \frac{\hbar\omega}{2}\left[\underbrace{\left(i\hat{\tilde{p}} + \hat{\tilde{x}}\right)}_{2^{1/2}\hat{\mathbf{a}}}\underbrace{\left(-i\hat{\tilde{p}} + \hat{\tilde{x}}\right)}_{2^{1/2}\hat{\mathbf{a}}^{\dagger}}\right]?$$

does this work? No, this attempt at factorization generates a term $i\left[\hat{\tilde{p}}, \hat{\tilde{x}}\right]$, which must be subtracted out: $\widehat{H} = \frac{\hbar\omega}{2}\left(2\hat{\mathbf{a}}\hat{\mathbf{a}} - i\underbrace{\left[\hat{\tilde{p}}, \hat{\tilde{x}}\right]}_{=-i}\right)$

$$\boxed{\begin{aligned}\hat{\mathbf{a}} &= 2^{-1/2}\left(\hat{\tilde{x}} + i\hat{\tilde{p}}\right)\\ \hat{\mathbf{a}}^{\dagger} &= 2^{-1/2}\left(\hat{\tilde{x}} - i\hat{\tilde{p}}\right)\\ \hat{\tilde{x}} &= 2^{-1/2}\left(\hat{\mathbf{a}} + \hat{\mathbf{a}}^{\dagger}\right)\\ \hat{\tilde{p}} &= i2^{-1/2}\left(\hat{\mathbf{a}}^{\dagger} - \hat{\mathbf{a}}\right)\end{aligned}}$$

be careful about $\left[\hat{\tilde{\mathrm{x}}},\hat{\tilde{\mathrm{p}}}\right] \neq 0$

We will find that

$$\hat{\mathbf{a}}\psi_{\mathrm{v}} = (v)^{1/2}\,\psi_{\mathrm{v}-1} \qquad \text{annihilates one quantum}$$
$$\hat{\mathbf{a}}^{\dagger}\psi_{\mathrm{v}} = (v+1)^{1/2}\,\psi_{\mathrm{v}+1} \qquad \text{creates one quantum}$$
$$\widehat{H} = \hbar\omega\left(\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger} - 1/2\right) = \hbar\omega\left(\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} + 1/2\right).$$

This is astonishingly convenient. It presages a form of operator algebra that proceeds without ever looking at the form of $\psi(x)$ and does not require <u>direct</u> evaluation of integrals of the form

$$A_{ij} = \int dx\ \psi_i^{*}\hat{A}\psi_j.$$

2. Now we must go back and repair our attempt to factor $\widehat{H}$ for the harmonic oscillator.

Instructive examples of operator algebra.

* What is $\left(i\hat{\tilde{p}} + \hat{\tilde{x}}\right)\left(-i\hat{\tilde{p}} + \hat{\tilde{x}}\right)$?

$$\hat{\tilde{p}}^2 + \hat{\tilde{x}}^2 + \underbrace{i\hat{\tilde{p}}\hat{\tilde{x}} - i\hat{\tilde{x}}\hat{\tilde{p}}}_{i\left[\hat{\tilde{p}},\hat{\tilde{x}}\right]}$$

Recall $\left[\hat{p},\hat{x}\right] = -i\hbar$. (work this out by $\hat{p}\hat{x}f - \hat{x}\hat{p}f = \left[\hat{p},\hat{x}\right]f$).

What is $i\left[\hat{\tilde{p}},\hat{\tilde{x}}\right]$?

$$\begin{aligned} i\left[\hat{\tilde{p}},\hat{\tilde{x}}\right] &= i[\hbar m\omega]^{-1/2}\left[\frac{\hbar}{m\omega}\right]^{-1/2}\left[\hat{p},\hat{x}\right]\\ &= i\left[\hbar^2\right]^{-1/2}(-i\hbar) = +1.\end{aligned}$$

So we were *not quite* successful in factoring $\widehat{H}$. We have to subtract (1/2)ħω:

$$\widehat{H} = \hbar\omega\left(\hat{\mathbf{a}}\widehat{\mathbf{a}^{\dagger}} - \underbrace{\frac{1}{2}}_{\substack{\text{left}\\ \text{over}}}\right)$$

This form for $\widehat{H}$ is going to turn out to be very useful.

* Another trick, what about $\left[\hat{\mathbf{a}},\hat{\mathbf{a}}^{\dagger}\right] = ?$

$$\left[\hat{\mathbf{a}},\widehat{\mathbf{a}^{\dagger}}\right] = \left[2^{-1/2}\left(i\hat{\tilde{p}} + \hat{\tilde{x}}\right), 2^{-1/2}\left(-i\hat{\tilde{p}} + \hat{\tilde{x}}\right)\right] = \frac{i}{2}\left[\hat{\tilde{p}},\hat{\tilde{x}}\right] + \frac{-i}{2}\left[\hat{\tilde{x}},\hat{\tilde{p}}\right]$$
$$= \frac{1}{2} + \frac{1}{2} = 1.$$

So we have some nice results. $\boxed{\hat{H} = \hbar\omega\left[\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} + \frac{1}{2}\right] = \hbar\omega\left[\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger} - \frac{1}{2}\right]}$

3. Now we will derive some amazing results *almost* without ever looking at a wavefunction.

If ψ_v is an eigenfunction of $\widehat{H}$ with energy E_v, then $\hat{\mathbf{a}}^\dagger\psi_v$ is an eigenfunction of $\widehat{H}$ belonging to eigenvalue $E_v + \hbar\omega$.

$$\widehat{H}\left(\widehat{a}^\dagger\psi_v\right) = \hbar\omega\left[\hat{a}^\dagger\hat{a} + \frac{1}{2}\right]\hat{a}^\dagger\psi_v$$

$$= \hbar\omega\left[\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \frac{1}{2}\hat{a}^\dagger\right]\psi_v$$

Factor $\hat{\mathbf{a}}^\dagger$ out front

$$= \hat{a}^\dagger\hbar\omega\left[\hat{a}\hat{a}^\dagger + \frac{1}{2}\right]\psi_v$$

$$\hat{a}\hat{a}^\dagger = \left[\hat{a},\hat{a}^\dagger\right] + \hat{a}^\dagger\hat{a} = 1 + \hat{a}^\dagger\hat{a}$$

$$\widehat{H}\left(\hat{a}^\dagger\psi_v\right) = \hat{a}^\dagger \underbrace{\hbar\omega\left[\hat{a}^\dagger\hat{a} + 1 + \frac{1}{2}\right]}_{\widehat{H}+\hbar\omega}\psi_v$$

and $\hat{H}\psi_v = E_v\psi_v$, thus

$$\widehat{H}\left(\hat{a}^\dagger\psi_v\right) = \hat{a}^\dagger\left(E_v + \hbar\omega\right)\psi_v = \left(E_v + \hbar\omega\right)\left(\hat{a}^\dagger\psi_v\right)$$

Therefore $\hat{\mathbf{a}}^\dagger\psi_v$ is eigenfunction of $\widehat{H}$ with eigenvalue $E_v + \hbar\omega$.

So every time we apply $\hat{\mathbf{a}}^\dagger$ to ψ_v, we get a new eigenfunction of $\widehat{H}$ and a new eigenvalue increased by $\hbar\omega$ from the previous eigenfunction. $\hat{\mathbf{a}}^\dagger$ *creates* one quantum of vibrational excitation.

Similar result for $\hat{\mathbf{a}}\,\psi_v$.

$$\widehat{H}\left(\hat{\mathbf{a}}\psi_v\right) = \left(E_v - \hbar\omega\right)\left(\hat{\mathbf{a}}\psi_v\right).$$

$\hat{\mathbf{a}}\,\psi_v$ is eigenfunction of $\widehat{H}$ that belongs to eigenvalue $E_v - \hbar\omega$. $\hat{\mathbf{a}}$ destroys one quantum of vibrational excitation.

We call $\hat{\mathbf{a}}^\dagger, \hat{\mathbf{a}}$ "ladder operators" or creation and annihilation operators (or step-up, step-down).

Now, suppose I apply $\hat{\mathbf{a}}$ to ψ_v many times. We know there must be a lowest energy eigenstate for the harmonic oscillator because $E_v \geq V(0)$.

We have a ladder and we know there must be a lowest rung on the ladder. If we try to step below the lowest rung we get

$$\hat{\mathbf{a}}\,\psi_{\min} = 0$$

$$2^{-1/2}\left[i\hat{\tilde{p}} + \hat{\tilde{x}}\right]\psi_{\min} = 0$$

$-i\hbar\frac{d}{dx}$

Now we bring $\hat{x}$ and $\hat{p}$ back.

$$\left[i(2\hbar\mu\omega)^{-1/2}\,\hat{p} + \left(\frac{\mu\omega}{2\hbar}\right)^{1/2}\hat{x}\right]\psi_{\min} = 0$$

$$\left[+\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\frac{d}{dx} + \left(\frac{\mu\omega}{2\hbar}\right)^{1/2} x\right]\psi_{\min} = 0$$

$$\frac{d\psi_{\min}}{dx} = -\left(\frac{2\mu\omega}{\hbar}\right)^{1/2}\left(\frac{\mu\omega}{2\hbar}\right)^{1/2} x\psi_{\min}$$

$$= -\frac{\mu\omega}{\hbar}x\psi_{\min}.$$

This is a first-order, linear, ordinary differential equation.

What kind of function has a first derivative that is equal to a negative constant times the variable times the function itself?

$$\frac{de^{-cx^2}}{dx} = -2cxe^{-cx^2}$$

$$c = \frac{\mu\omega}{2\hbar}$$

$$\psi_{\min} = N_{\min}e^{-\frac{\mu\omega}{2\hbar}x^2}.$$

(A Gaussian)

The lowest vibrational level has eigenfunction, $\psi_{\min}(x)$, which is a simple Gaussian, centered at $x = 0$, and with tails extending into the classically forbidden $E < V(x)$ regions.

Now normalize:

$$\int_{-\infty}^{\infty} dx\ \underbrace{\psi_{\min}^{*}\psi_{\min}}_{\substack{\text{give factor of}\\ \text{2 in exponent}}} = 1 = N_{\min}^{2}\ \underbrace{\int_{-\infty}^{\infty} dx\ e^{-\frac{\mu\omega}{\hbar}x^2}}_{\frac{\pi^{1/2}}{(\mu\omega/\hbar)^{1/2}}}$$

$$\boxed{\psi_{\min}(x) = \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{\mu\omega}{2\hbar}x^2}}$$

[recall asymptotic factor of $\psi(x)$: $e^{-\xi^2/2}$]

This is the lowest energy normalized wavefunction. It has zero nodes.

NON-LECTURE

Gaussian integrals

$$\int_0^{\infty} dx\ e^{-r^2x^2} = \frac{\pi^{1/2}}{2r}$$

$$\int_0^{\infty} dx\ xe^{-r^2x^2} = \frac{1}{2r^2}$$

$$\int_0^{\infty} dx\ x^2e^{-r^2x^2} = \frac{\pi^{1/2}}{4r^3}$$

$$\int_0^{\infty} dx\ x^{2n+1}e^{-r^2x^2} = \frac{n!}{2r^{2n+2}}$$

$$\int_0^{\infty} dx\ x^{2n}e^{-r^2x^2} = \pi^{1/2}\frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}r^{2n+1}}$$

By inspection, using dimensional analysis, all of these integrals seem OK.

We need to clean up a few loose ends.

1. Could there be several independent ladders built on linearly independent $\psi_{\min_1}$, $\psi_{\min_2}$?

   Assertion: for any 1-D potential it is possible to show that the energy eigenfunctions are arranged so that the quantum numbers increase in step with the number of internal nodes.

   particle in box n = 1, 2, …

   \# nodes = 0, 1, …, which translates into the general rule

   \# nodes = n – 1

   harmonic oscillator $v = 0, 1, 2, \ldots$

nodes = v

We have found a $\psi_{\min}$ that has zero nodes. It must be the lowest energy eigenstate. Call it $v = 0$.

2. What is the lowest energy? We know that energy increases in steps of $\hbar\omega$.

$$E_{v+n} - E_v = n\hbar\omega.$$

We get the energy of $\psi_{\min}$ by plugging $\psi_{\min}$ into the Schrödinger equation.

BUT WE USE A TRICK:

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

$$\widehat{H}\psi_{\min} = \hbar\omega\left(\widehat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} + \frac{1}{2}\right)\psi_{\min}$$

$$\text{but } \hat{\mathbf{a}}\psi_{\min} = 0$$

$$\text{so } \widehat{H}\psi_{\min} = \hbar\omega\left(0 + \frac{1}{2}\right)\psi_{\min}$$

$$E_{\min} = \frac{1}{2}\hbar\omega!$$

Now we also know

$$E_{\min+n} - E_{\min} = n\hbar\omega$$

OR

$$\mathrm{E}_{0+v} - E_0 = v\hbar\omega, \text{ thus } E_v = \hbar\omega(v + 1/2)$$

NON-LECTURE

3. We know

$$\hat{\mathbf{a}}^{\dagger}\psi_{\mathrm{v}} = c_{\mathrm{v}}\psi_{\mathrm{v}+1}$$
$$\hat{\mathbf{a}}\psi_{\mathrm{v}} = d_{\mathrm{v}}\psi_{\mathrm{v}-1}$$

what are c_{v} and d_{v}?

$$\widehat{H} = \hbar\omega\left(\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} + \frac{1}{2}\right) = \hbar\omega\left(\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger} - \frac{1}{2}\right)$$

$$\frac{\widehat{H}}{\hbar\omega} - \frac{1}{2} = \hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}, \quad \frac{\widehat{H}}{\hbar\omega} + \frac{1}{2} = \hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger}$$

$$\left(\frac{\widehat{H}}{\hbar\omega} - \frac{1}{2}\right)\psi_v = \left(v + \frac{1}{2} - \frac{1}{2}\right)\psi_v = \hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}\psi_v$$

$$\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}\,\psi_v = v\psi_v$$

$\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}$ is "number operator", $\widehat{N}$.

for $\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger}$ we use the trick

$$\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger} = \hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} + \underbrace{\left[\hat{\mathbf{a}}, \hat{\mathbf{a}}^{\dagger}\right]}_{+1} = \widehat{N} + 1$$

Now $\int dx\ \psi_{\mathrm{v}}^{*}\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger}\psi_{\mathrm{v}} = \int dx\left|\hat{\mathbf{a}}^{\dagger}\psi_{\mathrm{v}}\right|^2$ because $\hat{\mathbf{a}}\hat{\mathbf{a}}^{\dagger}$ is Hermitian

Prescription for operating to the left is $\psi_v^{*}\hat{\mathbf{a}} = \left(\hat{\mathbf{a}}^{*}\psi_v\right)^{*} = \left(\mathbf{a}^{\dagger}\psi_v\right)^{*}$

$$\mathrm{v} + 1 = \left|c_{\mathrm{v}}\right|^2$$

$$c_{\mathrm{v}} = [\mathrm{v} + 1]^{1/2}$$

similarly for d_v in $\hat{\mathbf{a}}\psi_v = d_v\psi_{v-1}$

$$\int dx\ \psi_v^{*}\hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}\psi_v = v$$

Make phase choice and then verify by putting in $\hat{x}$ and $\hat{p}$.

$$\int \mathrm{dx}\left|\hat{\mathbf{a}}\psi_v\right|^2 = \left|d_v\right|^2$$

$$d_{\mathrm{v}} = v^{1/2}$$

Again, verify phase choice

$$\boxed{\begin{aligned}&\hat{\mathbf{a}}^{\dagger}\psi_v = (v+1)^{1/2}\,\psi_{v+1}\\&\hat{\mathbf{a}}\psi_v = (v)^{1/2}\,\psi_{v-1}\\&\widehat{N} = \hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}}\\&\widehat{N}\psi_v = v\psi_v\\&\left[\hat{\mathbf{a}},\hat{\mathbf{a}}^{\dagger}\right] = 1\end{aligned}}$$

Remember these five exceptionally important equations!

Now we are ready to exploit the $\widehat{\mathbf{a}^{\dagger},\hat{\mathbf{a}}}$ operators.

Suppose we want to look at vibrational transition intensities.

use $\widehat{\hat{\mathbf{a}},\mathbf{a}^{\dagger}}$

$$\mu(x) = \mu_0 + \mu_1\hat{x} + \mu_2\hat{x}^2/2 + \ldots$$

More generally, suppose we want to compute an integral involving some integer power of $\hat{x}$ (or $\hat{p}$).

$$\hat{\mathbf{a}}^{\dagger} = 2^{-1/2}\left(-i\hat{\tilde{p}} + \hat{\tilde{x}}\right)$$

$$\hat{\mathbf{a}} = 2^{-1/2}\left(i\hat{\tilde{p}} + \hat{\tilde{x}}\right)$$

$$\widehat{N} = \hat{\mathbf{a}}^{\dagger}\hat{\mathbf{a}} \qquad \text{(number operator)}$$

$$\hat{\tilde{x}} = 2^{-1/2}(\hat{\mathbf{a}}^{\dagger} + \hat{\mathbf{a}})$$

$$\hat{\tilde{p}} = 2^{-1/2}i(\hat{\mathbf{a}}^{\dagger} - \hat{\mathbf{a}})$$

$$\hat{x} = \left[\frac{\mu\omega}{\hbar}\right]^{-1/2}\hat{\tilde{x}} = \left[\frac{2\mu\omega}{\hbar}\right]^{-1/2}(\hat{\mathbf{a}}^{\dagger} + \hat{\mathbf{a}})$$

$$\hat{p} = [\hbar\mu\omega]^{1/2}\,\hat{\tilde{p}} = \left[\frac{\hbar\mu\omega}{2}\right]^{1/2} i(\hat{\mathbf{a}}^{\dagger} - \hat{\mathbf{a}})$$

$$\widehat{x^2} = \frac{\hbar}{2\mu\omega}(\hat{\mathbf{a}}^\dagger + \hat{\mathbf{a}})(\hat{\mathbf{a}}^\dagger + \hat{\mathbf{a}}) = \frac{\hbar}{2\mu\omega}\left[\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 + \hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger\right] = \frac{\hbar}{2\mu\omega}\left[\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 + 2\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + 1\right]$$

$$\widehat{p^2} = -\frac{\hbar\mu\omega}{2}(\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 - \hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} - \hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger) = \frac{-\hbar\mu\omega}{2}\left[\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 - 2\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} - 1\right]$$

etc.

$$\widehat{H} = \frac{\widehat{p^2}}{2\mu} + \frac{k}{2}\widehat{x^2} = -\frac{\hbar\omega}{4}(\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 - 2\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} - 1) + \frac{\hbar\omega}{4}(\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2 + 2\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + 1) = \hbar\omega(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + 1/2)$$

as expected. The terms in $\widehat{H}$ involving $\hat{\mathbf{a}}^{\dagger 2} + \hat{\mathbf{a}}^2$ exactly cancel out.

Look at an $(\hat{\mathbf{a}}^\dagger)^m(\hat{\mathbf{a}})^n$ operator and, from $m - n$, read off the selection rule for Δv. Integral is not zero when the selection rule is satisfied.

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