One-Dimensional Problems Liboff chap. 7

In this chapter we're going to take another look at some 1-D problems we're familiar with from P237, especially the simple harmonic oscillator. In the S.H.O. case, we're going to solve the Schröodinger eq'n in a new way.

Properties of the 1-D Schröodinger Eq'n

First let's review some properties of the 1-D time-indep. Schr. eq'n (+ note that this is an eq'n for an energy eigenstate)

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

Recall that we can recast this as an eq'n for the curvature of the wave fn $\psi(x)$:

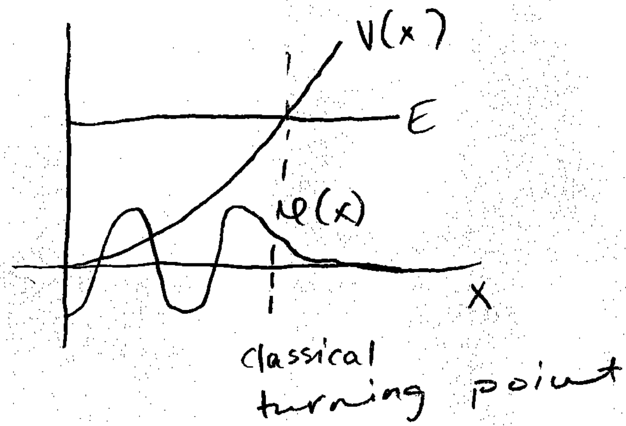
$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi(x)$$

Review the discussion of what this means for various signs of $V-E$, either in Liboff (~p. 189) or in your P237 book or notes. The upshot is.

$E > V$ = classically allowed region
$\Rightarrow$ oscillatory sol'ns

$E < V$ = classically disallowed region
$\Rightarrow$ ~exponential-type sol'ns (curvature away fr/ axis)

The situation is summarized in Fig. 7.3, for example. (6.2)



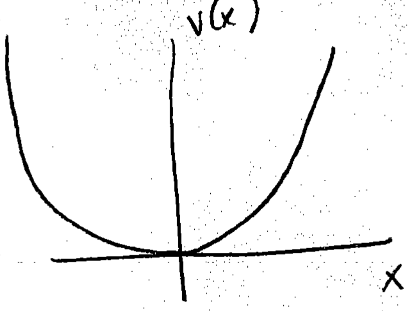
Simple harmonic oscillator

Recall that the S.H.O. is a good approximation for many physical systems, including most potentials with a minimum (think Taylor series expansion).

Some examples:

- vibrations of atoms in diatomic molecules
- acoustic + thermal properties of solids fr/ atomic vibrations
- magnetic properties of solids arising fr/ vibrations in orientations of nuclei
- electrodynamics of QM systems w/ vibrating EM waves

$$V(x) = \frac{1}{2} K x^2$$



Classically, eq'n of motion is Hooke's law;

spring const

$$m\frac{d^2x}{dt^2} = -Kx$$

and the angular frequency is

$$\omega_0 = \sqrt{\frac{K}{m}}$$

$$\Rightarrow \quad \frac{d^2x}{dt^2} + \omega_0^2 x = 0 \qquad (*)$$

Now we can immediately show that the energy is a constant of the motion by expressing the LHS as a total derivative Multiply (*) by $\dot{x} = \frac{dx}{dt}$:

$$\ddot{x}\dot{x} + \omega_0^2 x\dot{x} = 0 = \frac{d}{dt}\left[\frac{1}{2}\dot{x}^2 + \omega_0^2 x^2\right] = 0$$

$$\Rightarrow \frac{1}{2}\dot{x}^2 + \omega_0^2 x^2 = \text{const}$$

Multiply by the mass m and we have the energy:

$$E = \underbrace{\tfrac{1}{2}m\dot{x}^2}_{\text{Kinetic}} + \underbrace{\frac{K}{2}x^2}_{\text{potential}}$$

and the particle is only allowed in the region where $KE > 0$, i.e. $E > V$.

Quantum mechanically we have

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(x)$$

which gives the time-indep. S.E.

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + \frac{K}{2}x^2\varphi = E\varphi$$

Without solving this explicitly, we already know that for $E > V$ the sol'ns are oscillatory and for $E > V$ (large x) the sol'ns decay away.

• Asymptotic behavior

In fact we can solve for the asymptotic (large x) behavior explicitly. For large enough x, we have $\frac{1}{2}Kx^2 \gg E$ and so let's neglect E in the Schr. eq'n, which becomes

$$\frac{d^2\varphi}{dx^2} = \frac{mK}{\hbar^2}x^2\varphi = \frac{m^2\omega_0^2}{\hbar^2}x^2\varphi$$

and for convenience define

$$\beta^2 \equiv \frac{m\omega_0}{\hbar} \quad \text{(dimensions = length}^{-2}\text{)}$$

and

$$\xi \equiv \beta x, \text{ dimensionless}$$

and trading x for ξ in the Schr. eq'n:

$$\frac{d^2\varphi(x)}{dx^2} = \beta^4 x^2 \varphi(x)$$

$$\Rightarrow \quad \frac{d^2\varphi(\xi)}{d\xi^2} = \xi^2 \varphi$$

Now in this asymptotic domain, $\xi \gg 1$ and the sol'n is

$$\varphi \sim A e^{\pm \xi^2/2} = A e^{\pm (\beta x)^2/2}$$

(note that when we plug this into the Schr eq'n we get

$$\frac{d\varphi}{d\xi} = \pm \xi \varphi$$

$$\& \quad \frac{d^2\varphi}{d\xi^2} = \pm\varphi + \xi^2\varphi \simeq \xi^2\varphi \,)$$

Now the + sign here gives a sol'n that blows up for large x, & is therefore not normalizable.

So for large x,

$$\varphi \sim A e^{-\xi^2/2} = A e^{-(\beta x)^2/2}$$

• P237 sol'n method - review

This asymptotic form should ring a bell from P237.
Recall how we solved the SHO problem there:

$\longrightarrow$

We wrote

$$\psi(x) = \left[\psi(\text{large } x)\right] * \overbrace{\left[\text{What's left over}\right]}^{\text{call this } H}$$

$\psi(\text{large } x)$ was the asymptotic sol'n given on the previous page. We plugged the factorized ψ back into the original Schr. eq'n to get a differential eq'n for H. We expanded H in a power series in x and obtained a recursion rel'n for the coefficients in the power series. We found that for ψ to be finite, the series must be finite; truncation gave us an expression for the energy, $E = \hbar\omega(n + \frac{1}{2})$ where n is an integer. We built up wave fns from the recursion rel'ns. The resulting functions H_n were the Hermite polynomials

- <u>Algebraic sol'n: raising and lowering operators</u>

Now we're going to solve the SHO in a simpler, but more abstract way. It's so simple it almost seems like cheating, but it turns out to be well motivated by the mathematical theory of groups.

Consider the following combinations of $\hat{x}$ + $\hat{p}$:

$$\boxed{\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right)}$$

and its hermitian conjugate (recall $\hat{x}^+ = \hat{x}$ + $\hat{p}^+ = \hat{p}$)

$$\boxed{\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)}$$

These definitions don't look intuitive and they're not, but they'll wind up having simple interpretations when they act on wave fns. Note $\hat{a}$ + $\hat{a}^+$ are dimensionless, and $\hat{a}$ is not hermitian since $\hat{a}^+ \neq \hat{a}$.

Q: what is $[\hat{a}, \hat{a}^+]$? Recall $[\hat{x}, \hat{p}] = i\hbar$

A: $[\hat{a}, \hat{a}^+] = \frac{\beta^2}{2}\left\{\frac{-2i}{m\omega_0}[\hat{x}, \hat{p}]\right\}$ since $[\hat{x}, \hat{x}] = [\hat{p}, \hat{p}] = 0$

$= \beta^2 \frac{(-i)}{m\omega_0} \hbar$ and since (p.6.4) $\beta^2 = \frac{m\omega_0}{\hbar}$,

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

so $\hat{a}\hat{a}^+ = 1 + \hat{a}^+\hat{a}$

Interesting. But what does it all mean physically? Let's write the Hamiltonian in terms of $\hat{a}$ + $\hat{a}^+$. We need $\hat{x}$ + $\hat{p}$ $\longrightarrow$

$$\hat{a} + \hat{a}^+ = \beta\sqrt{2}\,\hat{x} \Rightarrow \hat{x} = \frac{\hat{a} + \hat{a}^+}{\beta\sqrt{2}}$$

$$a - a^+ = \beta\sqrt{2}\,\frac{i}{m\omega_0}\,\hat{p} \Rightarrow \hat{p} = -im\omega_0\,\frac{(\hat{a} - \hat{a}^+)}{\beta\sqrt{2}}$$

So substituting into $\hat{H}$,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = -\frac{m^2\omega_0^2}{2\beta^2 2m}(\hat{a} - \hat{a}^+)^2 + \frac{m\omega_0^2}{4\beta^2}(\hat{a} + \hat{a}^+)^2$$

$$= -\frac{m^2\omega_0^2\hbar}{4m\omega_0}(\hat{a} + \hat{a}^+)^2 + \frac{m\omega_0^2\hbar}{4m\omega_0}(\hat{a} + \hat{a}^+)^2$$

$$= \frac{\hbar\omega_0}{4}\,2(\hat{a}\hat{a}^+ + \hat{a}^+\hat{a})$$ and since $\hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1$

$$\boxed{\hat{H} = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)}$$

So now if we can find eigenfns + eigenvalues of $\hat{a}^+ a$, that solves the S.H.O.! We can. Let's do some labeling. Let

$$\hat{N} \equiv \hat{a}^+\hat{a}$$

with eigenfns ψ_n and eigenvalues n:

$$\hat{N}\psi_n = \hat{a}^+\hat{a}\,\psi_n = n\,\psi_n$$

We're using this notation because it will turn out that n is an integer. We don't know that yet, though, so for the time being it is just a number (a real one, since $\hat{N}$ is hermitian).

Now, we have to figure a few things out.

Q1: What does $\hat{a}$ mean physically? What does it do when acting on φ_n? To find out, operate on $\hat{a}\varphi$ with $\hat{N}$:

$$\hat{N}(\hat{a}\varphi_n) = \hat{a}^+\hat{a}(\hat{a}\varphi_n) = (\hat{a}\hat{a}^+ - 1)\hat{a}\varphi_n = \hat{a}(\hat{a}^+\hat{a} - 1)\varphi_n$$

$$= \hat{a}(N-1)\varphi_n = \hat{a}(n-1)\varphi_n = (n-1)\hat{a}\varphi_n$$

i.e. $\hat{N}(\hat{a}\varphi_n) = (n-1)\hat{a}\varphi_n$

which means $\hat{a}\varphi_n$ is an eigenfn of $\hat{N}$ w/ eigenvalue $n-1$:

$$\hat{a}\varphi_n = \text{const } \varphi_{n-1}$$

$$\hat{a}\varphi_{n-1} = \text{const } \varphi_{n-2} \quad \text{etc}$$

⇒ $\hat{a}$ is called a "lowering" or "annihilation" operator. "Lowering" because it changes the state to one w/ a lower eigenvalue. "Annihilation" for reasons we'll see later.

Q2: What does $\hat{a}^+$ mean physically?
A similar approach shows

$$\hat{N}\hat{a}^+\varphi_n = (n+1)\hat{a}^+\varphi_n$$

⇒ $\hat{a}^+\varphi_n$ is an eigenfn of $\hat{N}$ w/ eigenvalue $n+1$

$$\hat{a}^+\varphi_n = \text{const } \varphi_{n+1}$$

$\Rightarrow$ $\hat{a}^+$ is called a "raising" or "creation" operator.
Again, it's "raising" because it changes the state to one w/ a higher eigenvalue; "creation" we'll understand later.

More about eigenvalues of $\hat{N} = \hat{a}^+\hat{a}$

$$\hat{N}\varphi_n = n\varphi_n$$

Let's find out what we can about the eigenvalues n.

First, the Hamiltonian tells us something. Recall

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}K\hat{x}^2$$

= sum of squares of 2 hermitian operators

Hermitian op's must have real eigenvalues, and their squares must therefore be nonnegative.

This implies $\langle H \rangle \geq 0$

Since this must always be true, it must be true for the special case of an eigenstate of $\hat{N}$, so

$$\hat{H}\varphi_n = \hbar\omega_0(\hat{N}+\tfrac{1}{2})\varphi_n = \hbar\omega(n+\tfrac{1}{2})\varphi_n$$

and $\langle \varphi_n | \hat{H}\varphi_n \rangle = \hbar\omega_0(n+\frac{1}{2}) \geq 0$

$$\Rightarrow \quad n \geq -\frac{1}{2}$$

So any states that might correspond to $n \le -1/2$ must vanish. Recall that $\hat{a}\varphi_n \propto \varphi_{n-1}$. So the vanishing happens if there exists a state $\varphi_{n_{min}}$ with $n_{min} \le +\frac{1}{2}$ and

$$\hat{a}\,\varphi_{n_{min}} = 0$$

So let's assume this condition is satisfied; we will show below that there is a sol'n for such a state.

Well, we know what n_{min} is! How? Take

$$\hat{N}\varphi_{n_{min}} = \hat{a}^+\hat{a}\,\varphi_{n_{min}} = \underset{\substack{\uparrow \\ \text{since } \hat{a}\varphi_{n_{min}}=0}}{0} = 0\,\varphi_{n_{min}}$$

and since $\hat{N}\varphi_n = n\varphi_n$, $n_{min} = 0$

Now we can use $\hat{a}^+$ to find the other n's. We already showed

$$\hat{N}\cdot\hat{a}^+\varphi_n = (n+1)\,\hat{a}^+\varphi_n$$

so taking $n=1$,

$$\hat{N}\,(\hat{a}^+\varphi_0) = 1\,\hat{a}^+\varphi_0 = \varphi_1$$

Now take $\hat{a}^+\varphi_1$ & do the same exercise, + keep repeating. This shows that

$$\boxed{n = \text{integer}}$$

Now we immediately recover the energy eigenvalues;

$$\hat{H}\varphi_n = \hbar\omega_0 (n+\tfrac{1}{2})\varphi_n$$

$$\Rightarrow \quad \boxed{E_n = \hbar\omega_0 (n+1/2)} \qquad n = 0, 1, 2, \ldots$$

and that was a lot easier than solving the Schrödinger eq'n! Of course solving the Schrödinger eq'n also gives us the wave fns, which we don't have yet...

<u>SHO Eigenfunctions</u>

... but which we can construct w/ the raising and lowering operators.

First it's convenient to write the raising & lowering op's in terms of the dimensionless variable ξ

$$\xi = \beta x \qquad \beta = \sqrt{\frac{m\omega_0}{\hbar}} \qquad \frac{\partial}{\partial x} = \frac{\partial}{\partial(\xi/\beta)} = \beta\frac{\partial}{\partial\xi}$$

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta}{\sqrt{2}}\left(x + \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right) = \frac{\beta}{\sqrt{2}}\left(\frac{\xi}{\beta} + \frac{\hbar}{m\omega_0}\beta\frac{\partial}{\partial\xi}\right)$$

$$= \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right) = \hat{a}$$

similarly

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)$$

And $$\hat{a}^\dagger\hat{a} = \frac{1}{2}\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right) = \frac{1}{2}\left(\xi^2 - \frac{\partial^2}{\partial\xi^2} - \overbrace{\frac{\partial}{\partial\xi}\xi}^{1+\xi\frac{\partial}{\partial\xi}} + \xi\frac{\partial}{\partial\xi}\right)$$

$$= \frac{1}{2}\left(\xi^2 - \partial^2/\partial\xi^2 - 1\right)$$

So S.E. becomes

$$\hat{H}\psi = \hbar\omega_0\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right) = E\psi$$

$$\Rightarrow \frac{\hbar\omega_0}{2}\left(\xi^2 - \frac{\partial^2}{\partial\xi^2} - 1 + 1\right) = E\psi$$

or $$\frac{\partial^2\psi}{\partial\xi^2} + \left(\frac{2E}{\hbar\omega_0} - \xi^2\right)\psi = 0$$

... but we don't have to solve this eq'n.

To get the eigenfunctions we need only note that the ground state wave fn ψ_0 satisfies (cf p. 6.11)

$$\hat{a}\psi_0 = 0$$

or $$\frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right)\psi_0 = 0 \quad \text{i.e.} \quad \frac{\partial\psi_0}{\partial\xi} = -\xi\psi_0$$

we can rewrite this (with total derivatives) as

$$\frac{d\psi_0}{\psi_0} = -\xi\, d\xi$$

+ integrating (from $\xi = 0$ to $\xi = \xi$) $\Rightarrow$

+ with $\psi_0(0) \equiv A_0$,

$$\ln\left(\frac{\psi_0}{\psi_0(0)}\right) = -\frac{\xi^2}{2}$$

$$\psi_0(\xi) = A_0 e^{-\xi^2/2}$$

To find A_0 we perform the normalization integral

$$\int_{-\infty}^{\infty} \psi_0(\xi)\, d\xi = 1 \quad \Rightarrow \quad A_0 = \left(\frac{1}{\pi}\right)^{1/4}$$

In terms of x, we have $\psi_0(x) = B_0 e^{-(\beta x)^2/2}$ with $B_0 = \left(\frac{\beta^2}{\pi}\right)^{1/4}$

so

$$\varphi_0(\xi) = \left(\frac{1}{\pi}\right)^{1/4} e^{-\xi^2/2} \quad \text{and} \quad \boxed{\varphi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-(\beta x)^2/2}}$$

Now we just use the raising operator $\hat{a}^+$ to generate all the other energy eigenstates, because remember (p. 6.9)

$$\hat{a}^+ \varphi_n = \text{const}\ \varphi_{n+1}$$

The normalization comes out right with

$$\varphi_1 = \hat{a}^+ \varphi_0$$

$$\varphi_2 = \frac{1}{\sqrt{2}} \hat{a}^+ \varphi_1 = \frac{1}{\sqrt{2}} (\hat{a}^+)^2 \varphi_0$$

$$\varphi_n = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n \varphi_0$$ - see below for proof

In terms of ξ,

$$\varphi_1 = \frac{1}{\sqrt{2}} \frac{1}{\pi^{1/4}} \underbrace{\left(\xi - \frac{\partial}{\partial \xi}\right) e^{-\xi^2/2}}_{(\xi + \xi)\, e^{-\xi^2/2}}$$

$$= \left(\frac{1}{2\sqrt{\pi}}\right)^{1/2} 2\xi e^{-\xi^2/2}$$

and in general we have

$$\left(\xi - \frac{\partial}{\partial \xi}\right)^n e^{-\xi^2/2} = H_n(\xi) e^{-\xi^2/2}$$

Hermite polynomials, order n

So our sol'ns and energies are

$$\boxed{\begin{aligned} \psi_n &= A_n \mathcal{H}_n(\xi)\, e^{-\xi^2/2} \\ E_n &= \hbar\omega_0 (n + \tfrac{1}{2}) \end{aligned}}$$

... much easier than what we did in P237!

(Now we can show that given normalized ground state wave fn ψ_0, the excited states are indeed given by

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n \psi_0}$$

... it's simply a matter of getting the normalization right, i.e. to show $\int \psi_n^+ \psi_n \, d\xi = 1$

Here's how. (This is not in the textbook.) We'll do this in two steps: ① Assuming ψ_{n-1} is normalized, find normalization for ψ_n. ② Generalize to obtain expression for ψ_n in terms of ψ_0.

① Suppose ψ_{n-1} is properly normalized, i.e. $\langle \psi_{n-1} | \psi_{n-1} \rangle = 1$.
Let

$$\psi_n = \underset{\substack{\uparrow \\ \text{norm. const}}}{N_n}\, \hat{a}^+ \psi_{n-1}$$

and find N_n s.t. ψ_n is also normalized

Normalization condition on ψ_n:

$$1 = \langle \psi_n | \psi_n \rangle = |N_n|^2 \langle \hat{a}^+ \psi_{n-1} | \hat{a}^+ \psi_{n-1} \rangle = |N_n|^2 \langle \psi_{n-1} | \hat{a}\hat{a}^+ \psi_{n-1} \rangle$$

and $\hat{a}\hat{a}^+ = \hat{a}^+\hat{a} + 1 = \hat{N} + 1$

$$= |N_n|^2 \langle \psi_{n-1} | (\hat{N} + 1) \psi_{n-1} \rangle = |N_n|^2 n$$

$$\Rightarrow \quad N_n = \frac{1}{\sqrt{n}}$$

So $\varphi_n = \frac{1}{\sqrt{n}} \hat{a}^+ \varphi_{n-1}$

② Now generalize to get φ_n in terms of φ_0:

$$\varphi_n = \frac{1}{\sqrt{n}} a^+ \underbrace{\varphi_{n-1}}_{\frac{1}{\sqrt{n-1}} a^+ \varphi_{n-2}} = \frac{1}{\sqrt{n(n-1)}} (a^+)^2 \varphi_{n-2}$$

$$= \cdots = \frac{1}{\sqrt{n(n-1)\cdots(n-i+1)}} (a^+)^i \varphi_{n-i}$$

$$= \frac{1}{\sqrt{n(n-1)\cdots(1)}} (a^+)^n \varphi_0$$

$$\boxed{\varphi_n = \frac{1}{\sqrt{n!}} (a^+)^n \varphi_n}$$

End of proof

So $\hat{a}^+|\varphi_n\rangle = (n+1)^{1/2} |\varphi_{n-1}\rangle$ follows fr/ above

$\hat{a}|\varphi_n\rangle = n^{1/2} |\varphi_{n-1}\rangle$ shown in similar way

For simplicity we can use <u>notation</u> $|\varphi_n\rangle \equiv |n\rangle$

$$\Rightarrow \boxed{\begin{aligned} \hat{a}^+ |n\rangle &= \sqrt{n+1}\ |n+1\rangle \\ \hat{a}\ |n\rangle &= \sqrt{n}\ |n-1\rangle \end{aligned}}$$

Check consistency: $\hat{N}|n\rangle = \hat{a}^+\hat{a}|n\rangle = \sqrt{n}\ \hat{a}^+|n-1\rangle = \sqrt{n}\sqrt{n}\,|n\rangle$
$= n|n\rangle$ OK

and the $|n\rangle$ obey the orthonormality condition
$$\langle n|\ell\rangle = \delta_{n\ell}$$

some examples:

Ex $\langle x \rangle = \langle n|\hat{x}|n\rangle$ $\qquad \hat{x} = \frac{1}{\sqrt{2}\beta}(\hat{a}+\hat{a}^+)$

$$= \frac{1}{\sqrt{2}\beta}\langle n|\hat{a}+\hat{a}^+|n\rangle$$

$$= \frac{1}{\sqrt{2}\beta}\left[n^{1/2}\underbrace{\langle n|n-1\rangle}_{\to 0} + (n+1)^{1/2}\underbrace{\langle n|n+1\rangle}_{\to 0}\right]$$

$$= 0$$

Ex $\langle p \rangle = \langle n|\hat{p}|n\rangle = \frac{m\omega_0}{\sqrt{2}i\beta}\langle n|\hat{a}-\hat{a}^+|n\rangle = 0$ similarly

Correspondence Principle: We've been over this in detail in P237, so here I'll just remind you that the classical and quantum prob. densities are meant to correspond at large quantum no's. See the book for a nice derivation of the classical prob. density. The upshot is (see p. 205, fig. 7.11)