ECE/MAT 211A winter 07

Additional solutions

#7•6-2: Virial Theorem

To circumvent the question of what is the correct operator for the radial component of the momentum (see Problem #7•4-1), we write $\hat{r}\cdot\hat{p}$ in Cartesian coordinates:

$$\hat{r}\cdot\hat{p} = \hat{x}\,\hat{p}_x + \hat{y}\,\hat{p}_y + \hat{z}\,\hat{p}_z\ , \tag{1}$$

and we draw on the rule (7•3-14a) to handle the operator products,

$$\left[\hat{x}\,\hat{p}_x, \hat{H}\right] = \hat{x}\left[\hat{p}_x, \hat{H}\right] + \left[\hat{x}, \hat{H}\right]\hat{p}_x = \hat{x}\left[\hat{p}_x, V\right] + \frac{1}{2M}\left[\hat{x}, \hat{p}_x^{\,2}\right]\hat{p}_x\ . \tag{2}$$

With the help of the commutator relations (7•3-9a) and (7•3-17b), this simplifies to

$$\left[\hat{x}\,\hat{p}_x, \hat{H}\right] = \hat{x}\cdot\left(-i\hbar\frac{\partial V}{\partial x}\right) + \frac{i\hbar}{M}\hat{p}_x^{\,2}\ . \tag{3}$$

Adding the two Cartesian equivalents of this and returning to vector notation leads to the claimed form (7•6-34).

Consider next

$$\left\langle \Psi \middle| \left[\hat{r}\cdot\hat{p}, \hat{H}\right] \middle| \Psi \right\rangle = \left\langle \Psi \middle| (\hat{r}\cdot\hat{p})\,\hat{H} \middle| \Psi \right\rangle - \left\langle \Psi \middle| \hat{H}(\hat{r}\cdot\hat{p}) \middle| \Psi \right\rangle . \tag{4}$$

Because $\hat{H}$ is Hermitian, we may view it in the first term as operating to the right, on $|\Psi\rangle$, and in the second term as operation to the left, on $\langle\Psi|$. If $|\Psi\rangle$ is an eigenstate, both terms in (4) ten simplify to $\varepsilon\left\langle \Psi \middle| \hat{r}\cdot\hat{p} \middle| \Psi \right\rangle$ and cancel, as claimed in (7•6-35). Evidently, the expectation values of the two terms on the right-hand side of (7•6-34) for any eigenstate of $\hat{H}$ must also cancel, which implies (7•6-36).

If V(r) is spherically symmetric, V = V(r), the virial theorem reduces to

$$2\langle \varepsilon_{kin} \rangle = \left\langle r\frac{dV}{dr} \right\rangle . \tag{5a}$$

Similarly, for one-dimensional problems, V = V(x), we have

$$2\langle \varepsilon_{kin} \rangle = \left\langle x \frac{dV}{dx} \right\rangle \tag{5b}$$

where ε_{kin} is now a one-dimensional kinetic energy.

For power-law potentials, $V \propto r^n$ or $V \propto x^n$, (5a,b) simplify further to

$$2\langle \varepsilon_{kin} \rangle = n\langle \varepsilon_{pot} \rangle . \tag{6}$$

This is true even for negative exponents, provided the expectation values are finite. The relation (7•6-37) for the harmonic oscillator (regardless of dimensionality) and (7•6-38) for the hydrogen atom are just special cases of (6).

In cases of power law potentials it is often convenient to express $\langle \varepsilon_{kin} \rangle$ and $\langle \varepsilon_{pot} \rangle$ not relative to each other, but relative to the total energy eigenvalue:

$$\langle \varepsilon_{kin} \rangle = \frac{n}{2+n}\varepsilon \quad \text{and} \quad \langle \varepsilon_{pot} \rangle = \frac{2}{2+n}\varepsilon \tag{7a,b}$$

#13•1-1: Displaced Harmonic Oscillator

(a)

We substitute the dimensionless operators $\hat{Q}$ and $\hat{P}$ introduced in (10•1-6) and (10•1-10)

$$\hat{Q} = \frac{x}{L} = \frac{1}{\sqrt{2}} \cdot \left(\hat{a}^{+} + \hat{a}^{-} \right), \quad \hat{P} = \frac{L\hat{p}}{\hbar} = \frac{i}{\sqrt{2}} \cdot \left(\hat{a}^{+} - \hat{a}^{-} \right). \tag{1a,b}$$

where $L = \sqrt{\hbar / Mw}$ is again the natural unit of length of the oscillator, from (2•3-7). If we insert (1a,b) into (13•1-28), utilize the commutation relation (10•1-4) for the stepping operators, and define $Q_0 = x_0 / L$, then (13•1-28) may be re-arranged to read

$$\hat{H} = \frac{1}{2}\hbar w \cdot \left[(\hat{a}^{+}\hat{a}^{-} + \frac{1}{2}) - \frac{Q_0}{\sqrt{2}} \cdot (\hat{a}^{+} + \hat{a}^{-}) + \frac{Q_0^2}{2} \right] = \hbar w \cdot \left[\left(\frac{\hat{a}^{+} - Q_0}{\sqrt{2}} \right) \left(\frac{\hat{a}^{-} - Q_0}{\sqrt{2}} \right) + \frac{1}{2} \right]. \tag{2}$$

This is evidently of the desired form (13•1-29), with

$$\hat{b}^{+} = \hat{a}^{+} - \frac{Q_0}{\sqrt{2}} \quad \text{and} \quad \hat{b}^{-} = \hat{a}^{-} - \frac{Q_0}{\sqrt{2}} . \tag{3a,b}$$

By inspection, the commutation relations for the $\hat{b}$'s are the same as for the $\hat{a}$'s:

$$\left[\hat{b}^+,\hat{b}^-\right]=\left[\hat{a}^+,\hat{a}^-\right]=-1, \tag{4}$$

which means that the $\hat{b}$'s are stepping operators for the displaced oscillator.

(b)

The ground state $\left|0_d\right\rangle$ of the displaced oscillator must satisfy

$$\hat{b}^-\left|0_d\right\rangle=0 \quad \text{or} \quad \hat{a}^-\left|0_d\right\rangle=\frac{Q_0}{\sqrt{2}}\left|0_d\right\rangle. \tag{5}$$

(c)

This is the same as the condition (10•2-17a) for the quasi-classical oscillating state, except that C in (10•2-17a) is now given, not by (10•2-23),

$$C=\sqrt{\langle n\rangle}\cdot e^{i(wt+\alpha)}, \tag{6}$$

but by the time-independent value

$$C=\frac{Q_0}{\sqrt{2}}. \tag{7}$$

Hence we may simply take over the math of that earlier problem by replacing $\langle n\rangle$ in the earlier problem according to

$$\langle n\rangle\rightarrow\frac{Q_0^2}{2}, \tag{8}$$

setting $t=0$ and $\alpha=0$, and requesting that all expansion coefficients be real. From (10•2-32), then,

$$c_0^2=\frac{1}{n!}\left(\frac{Q_0^2}{2}\right)^n\cdot\exp\left(-\frac{Q_0^2}{2}\right). \tag{9}$$

and the displaced state itself is

$$\left|0_d\right\rangle=\sum_0^\infty c_n\left|n\right\rangle=\exp\left(-\frac{Q_0^2}{4}\right)\cdot\sum_0^\infty\frac{1}{\sqrt{n!}}\cdot\left(\frac{Q_0}{\sqrt{2}}\right)^n\left|n\right\rangle. \tag{10}$$

We saw in sec. 10.2.2 that the quasi-classical oscillating state is a rigidly oscillating Gaussian wave packet with the same shape as the ground state of the harmonic oscillator. Hence the ground state of the displaced oscillator is basically a snapshot of the quasi-classical state of the undisplaced oscillator, caught at a suitable instant of time.

Comment:

The higher energy eigenstates of the displaced oscillator are obtained by repeatedly applying the operator $\hat{b}^+$ to (10) and drawing on (3a) inside the sum on the right-hand side. For example,

$$\left|1_d\right\rangle = \hat{b}^+\left|0_d\right\rangle = \sum_0^\infty c_n \cdot \left(\hat{a}^+ - \frac{Q_0}{\sqrt{2}}\right)\left|n\right\rangle = \sum_0^\infty c_n \cdot \left(\sqrt{n+1}\cdot\left|n+1\right\rangle - \frac{Q_0}{\sqrt{2}}\left|n\right\rangle\right)$$

$$= \sum_0^\infty \left(c_{n-1}\sqrt{n} - c_n \frac{Q_0}{\sqrt{2}}\right)\left|n\right\rangle = \sum_0^\infty c_n \cdot \left(\frac{n\sqrt{2}}{Q_0} - \frac{Q_0}{\sqrt{2}}\right)\left|n\right\rangle. \quad (11)$$

Here, on the last line, we have first re-numbered the $\left|n+1\right\rangle$-terms and then used (10•2-28) to re-express c_{n-1} in terms of c_n.