Quantum Mechanics and Atomic Physics 750:361

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HW #6

1. Reed, Prob. 5-5

Verify by explicit calculation that the n = 0 and n = 2 harmonic oscillator wavefunctions are orthonormal.

The wavefunctions are

$$\psi_o(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\alpha^2 x^2/2}$$

and

$$\psi_2(x) = \sqrt{\frac{\alpha}{8\sqrt{\pi}}}\ (4\alpha^2 x^2 - 2)\ e^{-\alpha^2 x^2/2}.$$

Hence

$$\int_{-\infty}^{\infty} \psi_o(x)\psi_2(x)dx = \frac{\alpha}{\sqrt{8\pi}} \int_{-\infty}^{\infty} (4\alpha^2 x^2 - 2)e^{-\alpha^2 x^2} dx$$

$$= \frac{8\alpha^3}{\sqrt{8\pi}} \int_0^{\infty} x^2 e^{-\alpha^2 x^2} dx - \frac{4\alpha}{\sqrt{8\pi}} \int_0^{\infty} e^{-\alpha^2 x^2} dx$$

$$= \frac{8\alpha^3}{\sqrt{8\pi}} \left(\frac{\sqrt{\pi}}{4\alpha^3}\right) - \frac{4\alpha}{\sqrt{8\pi}} \left(\frac{\sqrt{\pi}}{2\alpha}\right) = 0.$$

2. Reed, Prob. 5-6

Consider a particle of mass m in the first excited state (n=1) of a harmonic oscillator potential. Compute the probability of finding the particle outside the classically allowed region.

Here we have

$$\psi_1(\xi) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}}\,(2\xi)\,e^{-\xi^2/2}.$$

The probability of finding the particle *within* the classically allowed region is given by

$$P_{in} = \int_{-x_{turning}}^{x_{turning}} \psi_1^*(x)\psi_1(x)\,dx = \frac{1}{\alpha}\int_{-\xi_{turning}}^{\xi_{turning}} \psi_1(\xi)\psi_1(\xi)\,d\xi.$$

Where we have used $\xi = \alpha x$. Given that the turning points of the motion in the n = 1 case are $\xi_{turning} = \pm\sqrt{3}$ (see problem 5-8 below) and that the integral is symmetric about $\xi = 0$, we have

$$P_{in} = \frac{4}{\sqrt{\pi}}\int_0^{\sqrt{3}} \xi^2\,e^{-\xi^2}\,d\xi,$$

The integral itself (apart from the factor of $4/\sqrt{\pi}$) evaluates to 0.393657. This gives P_{in} = 0.8884, or $P_{out} = 0.1116$.

3. Reed, Prob. 5-7

In the case of a diatomic molecule, the analysis of the harmonic potential proceeds as above but with the mass m replaced by the reduced mass of the molecule, $m_1 m_2/(m_1 + m_2)$, where m_1 and m_2 are the masses of the atoms. In the case of molecular hydrogen, H_2, the equal spacing between the vibrational levels corresponds to a linear frequency ν of $12.48 \times 10^{13}\ \mathrm{sec}^{-1}$. Determine the effective force constant k for H_2.

Define the reduced mass to be μ. For H_2, $\mu = m/2$ where m is the mass of an individual hydrogen atom, hence $\mu = 8.365 \times 10^{-28}$ kg.

The energy ΔE released in a $\Delta n = 1$ harmonic oscillator transition is

$$\Delta E = \hbar\omega = \hbar\sqrt{k/\mu}.$$

If ν is the frequency of the photon emitted during the transition then $\Delta E = 2\pi\hbar\nu$, or

$$k = 4\pi^2\mu\nu^2 = 4\pi^2\,(8.365 \times 10^{-28})(12.48 \times 10^{13})^2 = 514.3\ \mathrm{N/m}.$$

This would make a strong spring: a Newton is equivalent to about a quarter-pound of force; it would take about 40 pounds of force to stretch this molecular bond by one foot!

4. Reed, Prob. 5-17

Following the approach that led to equation (5.5.30), use the raising and lowering operators to show that $\langle p^2 \rangle = \alpha^2\hbar^2(n+1/2)$ for the n'th harmonic-oscillator state, and hence verify that $\Delta x \Delta p$ is as given in problem 5-10.

The momentum operator is

$$p_{op} = \frac{\alpha\hbar}{\sqrt{2}}(A^+ + A^-)$$

Operate this on harmonic-oscillator state n:

$$\langle p^2 \rangle = \int \psi_n(p_{op}^2\psi_n)dx = \frac{\alpha^2\hbar^2}{2}\int \psi_n[(A^+ + A^-)(A^+\psi_n + A^-\psi_n)]dx$$

$$= \frac{\alpha^2\hbar^2}{2}\int \psi_n(A^+A^+\psi_n + A^+A^-\psi_n + A^-A^+\psi_n + A^-A^-\psi_n)dx.$$

By orthogonality, only the second and third terms make non-zero contributions:

$$\langle p^2 \rangle = \frac{\alpha^2\hbar^2}{2}\int \psi_n(A^+A^-\psi_n + A^-A^+\psi_n)dx.$$

Just as in the calculation of $\langle x^2 \rangle$, the bracketed term is, but for a constant, the Hamiltonian operator:

$$\mathbf{H} \equiv \frac{\hbar\omega}{2}(A^-A^+ + A^+A^-),$$

hence

$$\langle p^2 \rangle = \frac{\alpha^2\hbar^2}{2}\frac{2}{\hbar\omega}\int \psi_n(\mathbf{H}\psi_n)dx = \frac{\alpha^2\hbar}{\omega}E_n = \alpha^2\hbar^2(n+1/2),$$

exactly as determined in Problem 5-10; $\Delta x \Delta p$ follows directly.

5. The energy of a harmonic oscillator energy eigenstate is given by E = (n+1/2)$\hbar\omega$. Using Virial theorem, show that <KE>=<PE>= (n+1/2)($\hbar\omega$/2) for the given state.

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$$2\langle KE\rangle = \langle x\frac{dV}{dx}\rangle = \langle m\omega^2 x^2\rangle$$

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

$$\Rightarrow \frac{dV}{dx} = m\omega^2 x$$

$$= 2\langle \frac{1}{2}m\omega^2 x^2\rangle = 2\langle V\rangle$$

$$\Rightarrow \langle KE\rangle = \langle V\rangle$$

Because $\langle E\rangle = \langle KE\rangle + \langle V\rangle$

$$= \langle KE\rangle + \langle KE\rangle$$

$$= 2\langle KE\rangle$$

$$\Rightarrow \langle KE\rangle = \langle V\rangle = \frac{1}{2}\langle E\rangle$$

$$= \frac{1}{2}\hbar\omega(n+\frac{1}{2})$$