PHY6938 Proficiency Exam Spring 2002
April 5, 2002
Modern Physics and Quantum Mechanics

1. Consider the Schrödinger equation for the linear harmonic oscillator,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi\,,$$

where m is the mass of the particle and ω is the angular frequency. The wavefunction and energy of the ground and first excited state are given by

$$\psi_{GS}(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\,\exp(-\alpha^2x^2/2)\,,\; E_{GS} = \frac{1}{2}\hbar\omega$$

$$\psi_{E1}(x) = \sqrt{\frac{\alpha}{2\sqrt{\pi}}}\,2\alpha x\exp(-\alpha^2x^2/2)\,,\; E_{E1} = \frac{3}{2}\hbar\omega\,,$$

respectively, where $\alpha = \sqrt{m\omega/\hbar}$. A perturbation term $H' = -m\omega^2 x x_0$ is added to the Hamiltonian of the harmonic oscillator.

The following integral may be useful:

$$\int_{-\infty}^{\infty} dx\, x^2\exp(-x^2) = \sqrt{\pi}/2$$

(a) Calculate the transition matrix element $\langle\psi_{GS}|H'|\psi_{E1}\rangle$.

$$\begin{aligned}
\langle\psi_{GS}|H'|\psi_{E1}\rangle &= -m\omega^2x_0\alpha^2\sqrt{\frac{2}{\pi}}\int_{-\infty}^{\infty} dx\; x^2\; \exp\left[-\alpha^2x^2\right]\\
&= [\text{change variable,}\quad x' = \alpha x]\\
&= -m\omega^2x_0\sqrt{\frac{2}{\pi}}\,\frac{1}{\alpha}\int_{-\infty}^{\infty} dx'\; x'^2\; \exp\left[-x'^2\right]\\
&= -m\omega^2x_0\sqrt{\frac{2}{\pi}}\,\frac{1}{\alpha}\,\frac{\sqrt{\pi}}{2}\\
&= -m\omega^2x_0\,\frac{1}{\alpha\sqrt{2}}\\
&= -m\omega^2x_0\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} \qquad (1)
\end{aligned}$$

(b) Obtain the ground state energy of the perturbed system to second order in H'.

From the perturbation theory, the energy of the system up to second order in perturbation is given by

$$E'_{GS} = E_{GS} + \langle\psi_{GS}|H'|\psi_{GS}\rangle + \frac{|\langle\psi_{GS}|H'|\psi_{E1}\rangle|^2}{E_{GS} - E_{E1}}. \quad (2)$$

Determine the second term in Eq.2. We obtain

$$\begin{aligned}
\langle\psi_{GS}|H'|\psi_{GS}\rangle &= -m\omega^2 \frac{\alpha}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx\, x\, \exp\left[-\alpha^2 x^2\right] \\
&= 0. \quad (3)
\end{aligned}$$

The reason is that the integral is over an symmetric interval. x is an odd function and $\exp\left[-\alpha^2 x^2\right]$ is an even function. This means that the integrand is odd function integrated over an symmetric interval. A very simple example would be integrating x over the $-1 \leq x \leq 1$.

Therefore the second term in Eq.2 is zero. The only contribution up to the second order comes from the third term. But we have calculated the expectation value in part (a). This means that

$$\begin{aligned}
E'_{GS} &= \frac{1}{2}\hbar\omega - \frac{1}{\hbar\omega}\, m^2\omega^4 x_0^2\, \frac{\hbar}{2m\omega} \\
&= \frac{1}{2}\hbar\omega - \frac{1}{2}m\omega^2 x_0^2. \quad (4)
\end{aligned}$$

(c) The perturbation is actually a displacement of the origin of the oscillator by x_0. Obtain the exact value of the ground state energy by completing the square in the potential energy term of $H + H'$ and compare your result to (b)

$$\begin{aligned}
H + H' &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - -m\omega^2 x x_0 \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x - x_0)^2 - \frac{1}{2}m\omega^2 x_0^2. \quad (5)
\end{aligned}$$

In Eq.5, if we can see that the first two terms define a harmonic oscillator, but it is different in that (i). the oscillator is centered at x_0; (ii) each state has a constant energy $\frac{1}{2}m\omega^2 x_0^2$ added to it. We can see that the results of the two parts are the same. Actually it can be shown that the matrix element of H' between the ground state and all other states except for the first excited state is zero.