

Jan 2000 #2 (QM)

$$H_0 = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V(\vec{r}_1) + V(\vec{r}_2)$$

$$V(\vec{r}) = \frac{1}{2}k r^2$$

$$H' = \epsilon(x_1 x_2 + y_1 y_2 - 2z_1 z_2)$$

Unperturbed Hamiltonian splits into 6 independent oscillators

$$\text{define } k \equiv m\omega^2$$

$$|\psi\rangle \rightarrow |n_{1x} n_{1y} n_{1z} n_{2x} n_{2y} n_{2z}\rangle, \quad E = 3\hbar\omega + \hbar\omega(n_{1x} + n_{1y} + n_{1z} + n_{2x} + n_{2y} + n_{2z})$$

Ground state is nondegenerate:  $|000000\rangle$

$$E'_n = \langle n^0 | H' | n^0 \rangle$$

$$E'_{gs} = \epsilon \langle 000000 | x_1 x_2 | 000000 \rangle + \dots$$

$$x_i = (a_{ix} + a_{ix}^\dagger) \frac{x_0}{\sqrt{2}} \quad x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

$x_i$  mixes the states; every term is 0 in  $E'_{gs}$

$$E_n^2 = \langle n^0 | H' | n^0 \rangle = \sum_{m \neq n} \frac{\langle n^0 | H' | m^0 \rangle \langle m^0 | H' | n^0 \rangle}{E_n^0 - E_m^0} = \sum_{m \neq n} \frac{|\langle n^0 | H' | m^0 \rangle|^2}{E_n^0 - E_m^0}$$

$$E_{gs}^2 = \sum_{n_{1x} \dots n_{2z} \neq 0} \frac{|\langle n_{1x} \dots n_{2z} | H' | 000000 \rangle|^2}{3\hbar\omega - (3\hbar\omega + \hbar\omega(n_{1x} + \dots + n_{2z}))}$$

$$= -\frac{\epsilon^2}{\hbar\omega} \sum_{n_{1x} \dots n_{2z}} \frac{|\langle n_{1x} \dots n_{2z} | x_1 x_2 + y_1 y_2 - 2z_1 z_2 | 000000 \rangle|^2}{n_{1x} + n_{1y} + n_{1z} + n_{2x} + n_{2y} + n_{2z}}$$

$$\text{First term: } \langle n_{1x} \dots n_{2z} | x_1 x_2 | 000000 \rangle \quad x_1 = \frac{x_0}{\sqrt{2}}(a_{1x} + a_{1x}^\dagger) \quad x_2 = \frac{x_0}{\sqrt{2}}(a_{2x} + a_{2x}^\dagger)$$

$$a|0\rangle = 0 \quad a^\dagger|0\rangle = |1\rangle$$

$$= \frac{x_0^2}{2} \langle n_{1x} \dots n_{2z} | 100100 \rangle = \frac{\hbar}{2m\omega} \delta_{1, n_{1x}} \delta_{1, n_{2x}} \delta_{0, \text{rest}}$$

$$\text{Similarly, Second term} = \frac{\hbar}{2m\omega} \delta_{1, n_{1y}} \delta_{1, n_{2y}} \delta_{0, \text{rest}}$$

$$\text{Third term} = -2 \left( \frac{\hbar}{2m\omega} \delta_{1, n_{1z}} \delta_{1, n_{2z}} \delta_{0, \text{rest}} \right)$$

$$E_{gs}^2 = -\frac{\epsilon^2 \hbar}{4m^2 \omega^3} \sum_{n_{1x} + \dots + n_{2z}} |A + B - 2C|^2 \quad \text{where } A=1 \text{ if } n_{1x}=1=n_{2x}, \text{ the rest}=0$$

$$B=1 \text{ if } n_{1y}=1=n_{2y}, \quad "$$

$$C=1 \text{ if } n_{1z}=1=n_{2z}, \text{ the rest}=0$$

$$(A+B-2C)^2 = (A+B)^2 - 2(A+B)(2C) + 4C^2$$

$$E_{gs}^2 = -\frac{e^2 \hbar}{4m^2 \omega^3} \sum_{n_i} \frac{A^2 + 2AB + B^2 - 4AC - 4BC + 4C^2}{n_{ix} + \dots + n_{iz}}$$

$A^2$  term:  $\frac{1}{2}$        $2AB$  term: 0; all cross terms vanish

$B^2$  term:  $\frac{1}{2}$

$4C^2$  term:  $4 \cdot \frac{1}{2} = 2$

$$E_{gs}^2 = \frac{-e^2 \hbar}{4m^2 \omega^3} \left[ \frac{1}{2} + \frac{1}{2} + 2 \right]$$

$$E_{gs}^2 = -\frac{3\hbar e^2}{4m^2 \omega^3}$$