Lecture 34 / Perturbation theory

Calculate the lowest order correction to the spectrum of an harmonic oscillator due to anharmonic terms.

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 +$$

$$\hat{V} = \varepsilon \alpha \frac{\hat{x}^3}{\lambda_q^3} + \varepsilon^2 \beta \frac{\hat{x}^4}{\lambda_q^4} = \hat{V}_3 + \hat{V}_4$$

To find corrections to energy levels, we have to determine the matrix elements

$\langle m | \hat{V} | n \rangle$ for the perturbation

Is there a correction linear in $\hat{V}_3$? no

Is there a correction to the first order? yes

$$\hat{x} = \frac{\lambda_q}{\sqrt{2}} \left(\hat{a}^+ + \hat{a} \right)$$

$$\hat{x}^3 = \frac{\lambda_q^3}{2^{3/2}} \left(a^{+2} + a^+ a + a a^+ + a a \right) \left(a^+ + a \right)$$

$$= \frac{\lambda_q^3}{2^{3/2}} \Big(a^{+3} + a^+ a a^+ + a a^+ a^+ + a a a^+ + a^{+2} a + a^+ a a + a a^+ a + a a a \Big)$$

34.2

$$\hat{x}^3|n\rangle = \frac{\lambda_q^3}{2^{3/2}}\Big(\sqrt{(n+1)(n+2)(n+3)}\,|n+3\rangle + \sqrt{(n+1)^3}\,|n+1\rangle$$

$$+\sqrt{(n+1)(n+2)^2}\,|n+1\rangle + (n+1)\sqrt{n}\,|n-1\rangle$$

$$+\; n\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,(n-1)\,|n-1\rangle$$

$$+\;\sqrt{n^3}\,|n-1\rangle + \sqrt{n(n-1)(n-2)}\,|n-3\rangle\Big)$$

$$= \frac{\lambda_q^3}{\sqrt{8}}\Big(\sqrt{(n+1)(n+2)(n+3)}\,|n+3\rangle + \sqrt{(n+1)}\cdot(n+1+n+2+n)\,|n+1\rangle$$

$$+\sqrt{n}\,((n+1)+n+n-1)\,|n-1\rangle + \sqrt{n(n-1)(n-2)}\,|n-3\rangle\Big)$$

$$= \frac{\lambda_q^3}{\sqrt{8}}\Big(\sqrt{(n+1)(n+2)(n+3)}\,|n+3\rangle + 3\sqrt{(n+1)^3}\,|n+1\rangle$$

$$+3\sqrt{n^3}\,|n-1\rangle + \sqrt{n(n-1)(n-2)}\,|n-3\rangle\Big)$$

$$\langle m|\hat{x}^3|n\rangle = \frac{\lambda_q^3}{\sqrt{8}}\Big[\sqrt{(n+1)(n+2)(n+3)}\,\delta_{m,n+3} +$$

$$3\sqrt{(n+1)^3}\,\delta_{m,n+1} + 3\sqrt{n^3}\,\delta_{m,n-1} + \sqrt{n(n-1)(n-2)}\,\delta_{m,n-3}\Big]$$

$$\Delta E^{(2)} = \frac{\varepsilon^2\alpha^2}{8}\left[-\frac{(n+1)(n+2)(n+3)}{3\hbar\omega} + \frac{9(n+1)^3}{\hbar\omega} + \frac{9n^3}{\hbar\omega} + \frac{n(n-1)(n-2)}{3\hbar\omega}\right]$$

$$= \frac{\varepsilon^2\alpha^2}{8\hbar\omega}\;\frac{\cancel{27n^3} + \cancel{n^3} - 3n^2 + 2n - \cancel{27n^3} - 81n^2 - 81n - 27 - \cancel{n^3} - 6n^2 - 11n - 6}{3}$$

34.3

$$\Delta E^{(2)}_{V_3} = -\frac{\varepsilon^2 \alpha^2}{8\hbar\omega}\,\frac{3n^2+81n^2+6n^2+2n+81n+11n+27+6}{3}$$

$$\cancel{= -\frac{\varepsilon^2\alpha^2}{4\hbar\omega}\left(3n^2+3n+\frac{3}{2}\right)}$$

$$= -\frac{\varepsilon^2\alpha^2}{8\hbar\omega}\frac{1}{3}\left[90n^2+90n+33\right]$$

$$= -\frac{15\varepsilon^2\alpha^2}{4\hbar\omega}\left(n^2+n+\frac{11}{30}\right).$$

What is about V_4? Because it contains ε^2, we can limit our consideration to the first order perturbation theory

$$\Delta E^{(1)}_{V_3} = \langle n | \hat{V}_4 | n \rangle$$

$$\hat{x}^4 = \lambda_4 \frac{\hat{x}^3}{\sqrt{2}}(a^+ + a) = \dots = \quad \text{we keep only } (a^+)^2 a^2 \text{ terms}$$

$$= \frac{\lambda_4^4}{4}\left(a^+ a a^+ a + a a^+ a^+ a + a a a^+ a^+ + a^{+2} a^2 + a^+ a a a^+ + a a^+ a a^+\right)$$

$$\langle n | x^4 | n \rangle = \frac{\lambda_4^4}{4}\left\{ n^2 + (n+1)n + (n+1)(n+2) + n(n-1) + (n+1)n + (n+1)^2\right)$$

34.4)

$$\langle n|\hat{x}^4|n\rangle = \frac{\lambda q^4}{4}\left(6n^2+[1+3-1+1+2]n+3\right)$$

$$= \frac{\lambda q^4}{4}\, 6\left(n^2+n+\frac{3}{2}\right)$$

$$\Delta E^{(1)}_{V_4} = \frac{3}{2}\left(n^2+n+\frac{3}{2}\right)\varepsilon^2\beta$$

$$E = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{15}{4}\frac{\varepsilon^2\alpha^2}{\hbar\omega}\left(n^2+n+\frac{11}{30}\right) + \frac{3}{2}\varepsilon^2\beta\left(n^2+n+\frac{3}{2}\right)$$

V_3 decreases levels, but V_4 pushes them up.

What is the effect of anharmonicity on wave functions?

$$C^{(1)}_{nm} = \frac{V_{mn}}{E_n^{(0)}-E_m^{(0)}}$$

$$\psi_n(x) = \psi_n^{(0)}(x) + \frac{\varepsilon\alpha}{\hbar\omega\sqrt{8}}\Bigg[\psi^{(0)}_{n+3}(x)\frac{\sqrt{(n+1)(n+2)(n+3)}}{-3}$$

$$+\psi^{(0)}_{n+1}(x)\;3(n+1)^{3/2}$$

$$+ 3\,\psi^{(0)}_{n-1}(x)\;n^{3/2} + \psi^{(0)}_{n-3}(x)\frac{\sqrt{n(n-1)(n-2)}}{3}\Bigg]$$

34.5

Response to electric field

$$\hat{V}_E = q\hat{x}\cdot E$$

$\langle n|\hat{x}|n\rangle = 0$

For an unperturbed oscillator $\delta W \propto E^2$,

$W = \vec{d}\cdot\vec{E}$; $\vec{d} \propto \chi E$, χ is the susceptibility

For an anharmonic oscillator

$\langle n | \hat{V}_E | n\rangle \neq 0$ because now

$\psi_n(x) = \psi_n^{(0)}(x) + \varepsilon\psi_{n\pm1}^{(0)}$

And the dipole moment is finite!