perturbation theory

- 5029 - nucleus finite size
- LHO $-x^2 + \cancel{\lambda x^4}$ perturbation - for which α is the ground state correction 0?
  (c.f. variational methods...) - or for which α is $\langle 2|V'|0\rangle = 0$
- degenerate case $e^{i\phi}, e^{-i\phi}$ with $\frac{L}{4}$ L ~~V_0~~ perturbation
  $\frac{L}{2}$ → no 1st order change since $\cos^2$ & $\sin^2$ have the same density there...
- ⋮ L/ hole → change potential to $\frac{1}{2} m\omega^2 x^2$

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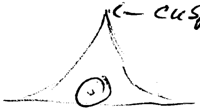
intro - chemistry, Feyn..., it's amazing - we can pretend that we know something about the system & calculate

H-like atom with Al core ($Z = 13$, $A = 27$) Al^{12+}

nucleus - uniformly charged sphere of radius ρ

compare energy difference between finite core and point charge on $|100\rangle$ state

→ result in eV & fraction of E_I of Al^{12+}



← cusp (jump in ψ'' to balance $\frac{1}{r} \to \frac{1}{0}$ singularity)

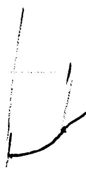
5029

feels only charge inside $< r$ volume

total volume $= \frac{4}{3}\pi\rho^3$, inside $r = \frac{4}{3}\pi r^3$

charge $= \frac{V_{ins}}{V_{tot}} = \frac{r^3}{\rho^3} \cdot 13$ or $\frac{r^3}{\rho^3} \cdot Z$

~~potential $= \frac{Ze^2}{4\pi\varepsilon_0 r} \cdot \frac{r^3}{\rho^3} + C$~~



- force $= -\frac{Ze^2}{4\pi\varepsilon_0 r^2} \cdot \frac{r^3}{\rho^3} = -\frac{Ze^2 r}{4\pi\varepsilon_0 \rho^3}$ $\quad F = -\frac{dV}{dx}$

potential $\int_0^r = +\frac{1}{2} \frac{Ze^2 r^2}{4\pi\varepsilon_0 \rho^3} + C$ ← below ρ

asymptotic potential $= -\frac{Ze^2}{4\pi\varepsilon_0 r}$

at ρ: $\frac{1}{2}\frac{Ze^2\rho^2}{4\pi\varepsilon_0 \rho^3} + C = -\frac{Ze^2}{4\pi\varepsilon_0 \rho}$

$$C = -\frac{3}{2}\frac{Ze^2}{4\pi\varepsilon_0 \rho} \quad ✓$$

$$\to V(r) = \frac{Ze^2}{4\pi\varepsilon_0}\left[\frac{1}{2}\frac{r^2}{\rho^3} - \frac{3}{2}\frac{1}{\rho}\right] \quad \text{for } r \leq \rho$$

$$-\frac{Ze^2}{4\pi\varepsilon_0 r} \quad \text{for } r \geq \rho$$

$\int u v\, dx = u\int v\, dx - \int u'\left(\int v\, dx\right)dx$

$\int \exp(-2Zr/a) = -\frac{a}{2Z}\exp(-2Zr/a)$

$\psi = \left(\frac{Z}{a}\right)^{3/2} \exp(-Zr/a) \cdot \sqrt{\frac{1}{4\pi}} \cdot 2$

$$\langle\psi|\psi\rangle = \frac{Z^3}{a^3} 4 \frac{1}{4\pi}\int d^3r \exp(-2Zr/a) = \frac{Z^3}{a^3}\frac{4}{\cancel{4\pi}}\cancel{4\pi}\int_0^\infty dr \exp(-2Zr/a)\cdot r^2 =$$

$$= \frac{4Z^3}{a^3}\left[\underbrace{r^2\cdot\left(-\frac{a}{2Z}\exp(-2Zr/a)\right)\Big|_0^\infty}_{=0} - \int_0^\infty dr\, 2r\left(-\frac{a}{2Z}\exp(-2Zr/a)\right)\right] =$$

$$= \frac{4Z^3}{a^3}\cdot 2\left(\frac{a}{2Z}\right)\left[\underbrace{r\left(-\frac{a}{2Z}\exp(-2Zr/a)\right)\Big|_0^\infty}_{=0} - \int_0^\infty\left(-\frac{a}{2Z}\exp(-2Zr/a)\right)dr\right] = \frac{8Z^3}{a^3}\frac{a^3(-)}{8Z^3}\exp\left(\frac{-2Zr}{a}\right)\Big|_0^\infty$$

$= 1$ OK

We have

$$\Psi = 2\cdot\left(\frac{Z}{a}\right)^{3/2}\sqrt{\frac{1}{4\pi}}\exp(-Zr/a)$$

$$H = H_0 + H'$$

$$H_0 = \frac{p^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 r} \qquad H' = \underbrace{+\frac{Ze^2}{4\pi\varepsilon_0 r}}_{-V_{orig}} + \underbrace{\frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{r^2}{2\rho^3} - \frac{3}{2\rho}\right)}_{V'} \quad \text{for } r \le \rho$$

$$H' = 0 \quad \text{for } r > \rho$$

$$\langle \Psi_{100} | H' | \Psi_{100} \rangle = \frac{4Z^3}{a^3}\frac{1}{4\pi}\int d^3r \exp(-2Zr/a)\left[\frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{1}{r} + \frac{r^2}{2\rho^3} - \frac{3}{2\rho}\right)\right]$$

$$= \frac{4Z^3}{a^3}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{4\pi}4\pi\int_0^\rho dr\, r^2\exp(-2Zr/a)\left[\frac{1}{r} + \frac{r^2}{2\rho^3} - \frac{3}{2\rho}\right]$$

Fermi model $r = r_0 A^{1/3}$ $r_0 = 1.2\cdot 10^{-15}\,m \rightarrow \rho = 3.6\cdot 10^{-15}\,m$

$$\exp\left(-2Z\cdot\frac{1.2\cdot 10^{-15}}{0.5\cdot 10^{-10}}\right) \approx \exp(-2\cdot 13\cdot 2.4\cdot 10^{-5}) \approx \exp(-6.5\cdot 10^{-4}) \approx 1$$

can be neglected

$$= \frac{4Z^4}{a^3}\frac{e^2}{4\pi\varepsilon_0}\int_0^\rho\left(r + \frac{r^4}{2\rho^3} - \frac{3r^2}{2\rho}\right)dr$$

$$= \frac{4Z^4}{a^3}\frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2}r^2 + \frac{1}{5}\frac{r^5}{2\rho^3} - \frac{1}{3}\frac{3r^3}{2\rho}\right]_0^\rho$$

$\rho = 3.6\,fm = 6.803\cdot 10^{-5}\,a.u.$

$$= \frac{4Z^4}{a^3}\frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2}\rho^2 + \frac{1}{10}\rho^2 - \frac{1}{2}\rho^2\right] = \frac{2}{5}\frac{Z^4}{a^3}\frac{e^2}{4\pi\varepsilon_0}\rho^2$$

in a.u. $= \frac{2}{5}Z^4\rho^2 = \frac{2}{5}\cdot 13^4\cdot(6.803\cdot 10^{-5})^2 = 5.287\cdot 10^{-5}$ a.u.

in eV $5.287\cdot 10^{-5}\cdot 27.2116 = 0.0014$ eV

for H-like atom, $E_I = \frac{Z^2e^2}{a\,4\pi\varepsilon_0}$, in a.u. $\rightarrow Z^2$ ← 1/2 missing in Lim! or result in Ry:...

Wiki: $E_I = \frac{Z^2 m e^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{1}{n^2} = \frac{Z^2e^2}{4\pi\varepsilon_0}\cdot\frac{me^2}{4\pi\varepsilon_0\hbar^2}\cdot\frac{1}{2}\cdot\frac{1}{n^2} =$

$a = \frac{\hbar^2 4\pi\varepsilon_0}{me^2}$

$$= \frac{Z^2e^2}{4\pi\varepsilon_0}\cdot\frac{1}{a}\cdot\frac{1}{2}\cdot\frac{1}{n^2} \overset{a.u.}{=} \frac{Z^2}{2n^2} = \frac{Z^2}{2}$$

for ground state

for ^{13}Al $= 169/2$ a.u. $= 84.5$ a.u.

$$\frac{\Delta E}{E_I} = \frac{5.287\cdot 10^{-5}}{84.5} = 6.26\cdot 10^{-7}$$

I guess spectroscopy ok with that?...

~~LHO with~~ Ax^6 from LHO

we have $H = \frac{p^2}{2m} + Ax^6$ ← we don't have this

estimate ground state energy

– use LHO: $H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

and $H' = -\frac{1}{2} m\omega^2 x^2 + Ax^6$

$\psi_0 = \left(\frac{a}{\pi}\right)^{1/4} e^{-\frac{ax^2}{2}} \qquad a = \frac{m\omega}{\hbar} \qquad \omega^2 = \frac{a^2\hbar^2}{m^2}$

$\langle 0 | H_0 | 0 \rangle = \frac{1}{2}\hbar\omega$

$\Delta \mathcal{E}_0 = \langle 0 | H' | 0 \rangle = \left(\frac{a}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx \left(-\frac{1}{2} m\omega^2\right) x^2 \exp(-ax^2) + \left(\frac{a}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx\, Ax^6 \exp(-ax^2)$

$= -\frac{1}{2} m\omega^2 \left(\frac{a}{\pi}\right)^{1/2} \frac{1}{2a} \sqrt{\frac{\pi}{a}} + A\left(\frac{a}{\pi}\right)^{1/2} \frac{5}{2a}\frac{3}{2a}\frac{1}{2a}\sqrt{\frac{\pi}{a}}$

$= -\frac{1}{2} m\omega^2 \cdot \frac{1}{2}\frac{\hbar}{m\omega} + A \cdot \frac{15}{8a^3} = -\frac{1}{4}\hbar\omega + \frac{15A}{8a^3}$

$= -\frac{1}{4}\frac{a\hbar^2}{m} + \frac{15A}{8a^3}$

$\langle 0 | H_0 + H' | 0 \rangle = \frac{1}{4}\hbar\omega + \frac{15A}{8a^3}$ or $= \frac{1}{4}\frac{a\hbar^2}{m} + \frac{15A}{8a^3}$ → we got this in variational ~~eval.~~ methods as a start

$\langle 2 | H' | 0 \rangle = 0$ condition ← no change in wavefunction of ground state through 2nd order

$a \to 2a$ there

$\psi_2 = \left(\frac{a}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2ax^2 - 1) e^{-ax^2/2}$

$\langle 2 | H' | 0 \rangle = \sqrt{\frac{a}{\pi}} \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} dx\, (2ax^2 - 1) Ax^6 e^{-ax^2} = \sqrt{\frac{a}{\pi}} \frac{A}{\sqrt{2}} 2a \int_{-\infty}^{\infty} dx\, x^8 e^{-ax^2} - \sqrt{\frac{a}{\pi}} \frac{A}{\sqrt{2}} \int_{-\infty}^{\infty} dx\, x^6 e^{-ax^2}$

$= \sqrt{\frac{a}{\pi}} \frac{A}{\sqrt{2}} 2a \cdot \frac{7}{2a}\frac{5}{2a}\frac{3}{2a}\frac{1}{2a}\sqrt{\frac{\pi}{a}} - \sqrt{\frac{a}{\pi}} \frac{A}{\sqrt{2}} \frac{5}{2a}\frac{3}{2a}\frac{1}{2a}\sqrt{\frac{\pi}{a}} =$

$= \frac{A}{\sqrt{2}} \frac{105}{8a^3} - \frac{A}{\sqrt{2}} \frac{15}{8a^3} = \frac{90A}{\sqrt{2}\, 8a^3}$ ← always finite change!

$\Delta \mathcal{E}_2 = \langle 2 | H' | 2 \rangle = \left(\frac{a}{\pi}\right)^{1/2} \left(-\frac{1}{2} m\omega^2\right) \int_{-\infty}^{\infty} dx\, x^2 (2ax^2 - 1)^2 \exp(-ax^2) + \left(\frac{a}{\pi}\right)^{1/2} A \int_{-\infty}^{\infty} dx\, x^6 (2ax^2 - 1)^2 \exp(-ax^2)$

$= \left(\frac{a}{\pi}\right)^{1/2} \left(-\frac{1}{2} m\omega^2\right) \int_{-\infty}^{\infty} x^2 (4a^2x^4 - 4ax^2 + 1) \exp(-ax^2)\, dx + \left(\frac{a}{\pi}\right)^{1/2} A \int_{-\infty}^{\infty} x^6 (4a^2x^4 - 4ax^2 + 1) \exp(-ax^2)$

$= \left(\frac{a}{\pi}\right)^{1/2} \left(-\frac{1}{2} m\omega^2\right) \left[4a^2 \frac{5}{2a}\frac{3}{2a}\frac{1}{2a}\sqrt{\frac{\pi}{a}} - 4a \frac{3}{2a}\frac{1}{2a}\sqrt{\frac{\pi}{a}} + \frac{1}{2a}\sqrt{\frac{\pi}{a}} \right] + \cancel{\left(\frac{a}{\pi}\right)^{1/2} A}$

$+ \left(\frac{a}{\pi}\right)^{1/2} A \left[4a^2 \frac{9 \cdot 5 \cdot 7 \cdot 3 \cdot 1}{4a^2 \cdot 8a^3} \sqrt{\frac{\pi}{a}} - 4a \frac{7 \cdot 5 \cdot 3 \cdot 1}{2a \cdot 8a^3} \sqrt{\frac{\pi}{a}} + \frac{5 \cdot 3 \cdot 1}{8a^3} \sqrt{\frac{\pi}{a}} \right]$

$= \left(-\frac{1}{2} m\omega^2\right) \left[\frac{15}{2a} - \frac{3 \cdot 2}{a \cdot 2} + \frac{1}{2a} \right] + A \left[\frac{9 \cdot 7 \cdot 5 \cdot 3}{8a^3} - \frac{7 \cdot 5 \cdot 3 \cdot 2}{4a^3 \cdot 2} + \frac{15}{8a^3} \right]$

$= \left(-\frac{1}{2} m\omega^2\right) \left[\frac{5}{2a} \right] + A \cdot \frac{375}{4a^3} = \left(-\frac{5}{4}\frac{a\hbar^2}{m}\right) + A \cdot \frac{375}{4a^3}$

the same shift $-\frac{1}{4}\frac{a\hbar^2}{m} + \frac{15A}{8a^3} = -\frac{5}{4}\frac{a\hbar^2}{m} + \frac{750A}{8a^3}$

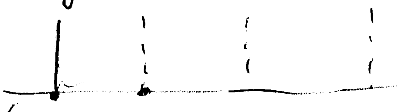
$\frac{8a^4\hbar^2}{m} = 735A$ vs $\frac{2a^4\hbar^2}{m} = 45A$

degenerate case

TS(8)

$\leftarrow$ particle in a periodic box (can be also in a circle)

wavefun $H = \frac{p^2}{2m}$



L

$\psi \sim e^{ixk} \qquad k = \frac{2\pi}{L} \cdot n \quad$ to be periodic

$\psi \sim e^{\frac{2\pi i x}{L} \cdot n}$

$\langle \psi | \psi \rangle = N^2 \int_0^L e^{\frac{2\pi i x n}{L}} \cdot e^{-\frac{2\pi i x n}{L}} dx = N^2 \int_0^L e^0 dx = N^2 \, x|_0^L = N^2 L = 1$

$N = \sqrt{\frac{1}{L}}$

$n = 0 \quad \varepsilon = 0 \quad \psi_0 = \sqrt{\frac{1}{L}}$

$n = 1$

$\sqrt{\frac{1}{L}} e^{\frac{i 2\pi x}{L}} \quad -\frac{\hbar^2}{2m}\frac{d}{dx^2} \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} e^{\frac{2\pi i x}{L}} = -\frac{\hbar^2}{2m}\left(2\pi i/L\right)^2 e^{\frac{2\pi i x}{L}}$

$= +\frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 e^{\frac{2\pi i x}{L}}$

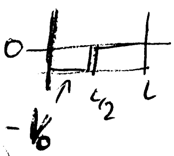
$\langle 1 | H | 1 \rangle = \frac{1}{L}\int_0^L e^{-\frac{2\pi i x}{L}} \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 e^{\frac{2\pi i x}{L}} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \frac{1}{L}\int_0^L 1 dx =$

$= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2$ or $\frac{\hbar^2 k^2}{2m}$

the same for $n = -1$

$\rightarrow$ twice degenerate

test potential



$\langle 1 | -V_0 | 1 \rangle = \frac{1}{L}\int_0^{L/2} e^{-\frac{2\pi i x}{L}} (-V_0) e^{\frac{2\pi i x}{L}} = \frac{1}{L}\int_0^{L/2} (-V_0) = -\frac{V_0}{2}$

$\langle -1 | -V_0 | -1 \rangle = -\frac{V_0}{2}$

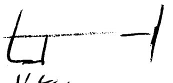
$\langle 1 | -V_0 | -1 \rangle = \frac{1}{L}\int_0^{L/2} e^{-\frac{2\pi i x}{L}} (-V_0) e^{-\frac{2\pi i x}{L}} =$

$\int e^{ax} = \frac{1}{a} e^{ax}$

$= \frac{1}{L}\int_0^{L/2} (-V_0) e^{-\frac{4\pi i x}{L}} = -\frac{V_0}{L} \left. \frac{e^{-\frac{4\pi i x}{L}}}{-\frac{4\pi i}{L}} \right|_0^{L/2}$

$= -\frac{V_0}{L}\left(\frac{L i}{4\pi}\right) e^{-\frac{4\pi i x}{L}}\Big|_0^{L/2} = -\frac{V_0 i}{4\pi}\left(e^{-2\pi i} - 1\right) = -\frac{V_0 i}{4\pi}(1-1) = 0$

$\langle -1 | -V_0 | 1 \rangle = 0$? higher order ? 2nd ???



$-V_0 \; L/4$

$\langle 1 | -V_0 | 1 \rangle = -\frac{V_0}{4}$

$\langle 1 | -V_0 | -1 \rangle = \frac{1}{L}\int_0^{L/4} dx \, e^{-\frac{2\pi i x}{L}} (-V_0) e^{-\frac{2\pi i x}{L}} = -\frac{V_0}{L}\int_0^{L/4} dx \, e^{-\frac{4\pi i x}{L}} =$

$= -\frac{V_0}{L}\frac{L}{-4\pi i} e^{-\frac{4\pi i x}{L}}\Big|_0^{L/4} = -\frac{i V_0}{4\pi}\left(\underset{-1}{e^{-i\pi}} - 1\right) = +\frac{i V_0}{2\pi}$

$\langle -1 | -V_0 | 1 \rangle = \frac{1}{L}\int_0^{L/4} dx \, e^{\frac{2\pi i x}{L}} (-V_0) e^{\frac{2\pi i x}{L}} = -\frac{V_0}{L}\int_0^{L/4} dx \, e^{\frac{4\pi i x}{L}} =$

$= -\frac{V_0}{L}\frac{L}{4\pi i} e^{\frac{4\pi i x}{L}}\Big|_0^{L/4} = \frac{i V_0}{4\pi}\left(\underset{-1}{e^{i\pi}} - 1\right) = -\frac{i V_0}{2\pi}$

so that in $|1\rangle$, $|-1\rangle$ basis, we have

$$\begin{array}{c|cc} & |1\rangle & |-1\rangle \\ \hline \langle 1| & -\frac{V_0}{4} & -\frac{iV_0}{4\pi}(e^{-i\pi}-1) \\ \langle -1| & \frac{iV_0}{4\pi}(e^{i\pi}-1) & -\frac{V_0}{4} \end{array} - \lambda I = 0$$

needs to be solved

or $\lambda I - \langle a|V|b\rangle = 0$

$e^{i\pi} = -1$
$e^{-i\pi} = -1$

$$\begin{vmatrix} \lambda + \frac{V_0}{4} & +\frac{iV_0}{4\pi}(e^{-i\pi}-1) \\ -\frac{iV_0}{4\pi}(e^{i\pi}-1) & \lambda + \frac{V_0}{4} \end{vmatrix} = 0$$

$$\left(\lambda + \frac{V_0}{4}\right)^2 + \left(\frac{iV_0}{4\pi}\right)^2 (e^{i\pi}-1)(e^{-i\pi}-1) =$$

$$= \lambda^2 + \frac{\lambda V_0}{2} + \frac{V_0^2}{16} - \frac{V_0^2}{16\pi^2}\left(1 + 1 - e^{i\pi} - e^{-i\pi}\right) =$$

$$= \lambda^2 + \frac{\lambda V_0}{2} + \frac{V_0^2}{16} - \frac{V_0^2}{8\pi^2}\left(1 - \frac{e^{i\pi}+e^{-i\pi}}{2}\right)$$

$$\begin{array}{c|cc} & |1\rangle & |-1\rangle \\ \hline \langle 1| & -\frac{V_0}{4} & +\frac{iV_0}{2\pi} \\ \langle -1| & -\frac{iV_0}{2\pi} & -\frac{V_0}{4} \end{array}$$

$\lambda I - \langle a|V_0|b\rangle$

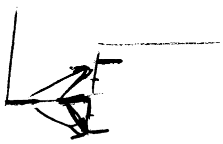
$$\begin{vmatrix} \lambda + \frac{V_0}{4} & -\frac{iV_0}{2\pi} \\ +\frac{iV_0}{2\pi} & \lambda + \frac{V_0}{4} \end{vmatrix} = 0$$

$$\lambda^2 + \frac{\lambda V_0}{2} + \frac{V_0^2}{16} - \left(-\frac{iV_0}{2\pi}\right)\left(\frac{iV_0}{2\pi}\right) = \lambda^2 + \frac{\lambda V_0}{2} + \frac{V_0^2}{16} - \frac{V_0^2}{4\pi^2}$$

$$b^2 - 4ac = \frac{V_0^2}{4} - 4 \cdot V_0^2\left(\frac{1}{16} - \frac{1}{4\pi^2}\right) = \frac{V_0^2}{4} - \frac{V_0^2}{4} + \frac{V_0^2}{\pi^2}$$

$$\cancel{\lambda_{1,2} = \frac{-b \pm \sqrt{D}}{2a} = -\frac{\lambda}{2} \pm \sqrt{\frac{\lambda^2}{4} - 4V_0^2\left(\frac{1}{16} - \frac{1}{4\pi^2}\right)}}$$

$$\lambda_{1,2} = \frac{-\frac{V_0}{2} \pm \frac{V_0}{\pi}}{2} = -\frac{V_0}{4} \pm \frac{V_0}{2\pi}$$



$$\left(\lambda_1 I - \langle a|V|b\rangle\right)|\psi_1\rangle = 0$$

$$\begin{pmatrix} \frac{V_0}{2\pi} & -\frac{iV_0}{2\pi} \\ +\frac{iV_0}{2\pi} & \frac{V_0}{2\pi} \end{pmatrix}|\psi_1\rangle = 0 \quad |\psi_1\rangle = \begin{pmatrix} 1 \\ -i \end{pmatrix} \quad |\psi_2\rangle = \begin{pmatrix} 1 \\ +i \end{pmatrix} \quad \text{ok}$$

$\psi_1 = \begin{pmatrix}1\\-i\end{pmatrix}^{|1\rangle}_{|-1\rangle}$ $\psi_2 \begin{pmatrix}1\\+i\end{pmatrix}^{|1\rangle}_{|-1\rangle}$ where $|1\rangle = e^{\frac{2\pi i x}{L}}\sqrt{\frac{1}{L}}$ $|-1\rangle = e^{-\frac{2\pi i x}{L}}\sqrt{\frac{1}{L}}$ T5(10)

$$\psi_1 = e^{\frac{2\pi i x}{L}} - i\, e^{-\frac{2\pi i x}{L}} = \cos\left(\frac{2\pi x}{L}\right) + i \sin\left(\frac{2\pi x}{L}\right) - i\cos\left(\frac{2\pi x}{L}\right) + i i \sin\left(\frac{2\pi x}{L}\right)$$

$e^{ix} = \cos x + i \sin x$
$$= (1-i)\cos\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)(-1+i) =$$
$$= (1-i)\left(\cos\left(\frac{2\pi x}{L}\right) - \sin\left(\frac{2\pi x}{L}\right)\right)$$

$$\psi_2 = e^{\frac{2\pi i x}{L}} + i\, e^{-\frac{2\pi i x}{L}} = \cos\left(\frac{2\pi x}{L}\right) + i \sin\left(\frac{2\pi x}{L}\right) + i\cos\left(\frac{2\pi x}{L}\right) - i \cdot i \sin\left(\frac{2\pi x}{L}\right)$$

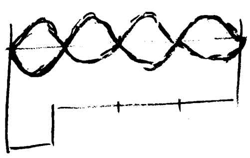
DU
$$= (1+i)\left(\cos\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)\right)$$

$$\psi_1^* \psi_1 = \cancel{\langle\psi_1|\psi_1\rangle} = (1-i)(1+i)\left(\cos\left(\frac{2\pi x}{L}\right) - \sin\left(\frac{2\pi x}{L}\right)\right)^2$$
$$= (1-i^2)\left[\cos^2\left(\frac{2\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right) - 2\cos\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\right]$$
$$= 2 \cdot \left[1 - 2\cos\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\right] = 2\left[1 - \sin\left(\frac{4\pi x}{L}\right)\right]$$

$$\psi_2^* \psi_2 = (1+i)(1-i)\left(\cos\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)\right)$$

~~looks odd~~ ...
looks OK

$$= 2 \cdot \left[1 + \sin\left(\frac{4\pi x}{L}\right)\right]$$



OK

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$$

$$V' = Ax = A\sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+)$$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \underbrace{\frac{1}{2} m\omega^2 x^2 + Ax}$$

$$\underset{a^2}{\frac{1}{2} m\omega^2 x^2} + \underset{2ab}{Ax} = \left(\sqrt{\frac{m}{2}}\,\omega x + \frac{A}{\sqrt{2m}\,\omega}\right)^2 - \frac{A^2}{2m\omega^2}$$

$$a = \frac{1}{\sqrt{2}}\sqrt{m}\,\omega \qquad 2ab = \cancel{2}\cdot 2\; A$$

$$2\cdot\frac{1}{\sqrt{2}}\sqrt{m}\,\omega\cdot b = A \Rightarrow b = \frac{A}{\sqrt{2m}\,\omega}$$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\Big(\sqrt{\frac{m}{2}}\,\omega x + \underbrace{\frac{A}{\sqrt{2m}\,\omega}}_{\text{change of mean}}\Big)^2 - \underbrace{\frac{A^2}{2m\omega^2}}_{\text{const. E shift}}$$

$$\langle n|V'|n\rangle = A\sqrt{\frac{\hbar}{2m\omega}}\,\langle n|a + a^+|n\rangle = 0$$

$$\langle m|V'|n\rangle = A\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|a + a^+|n\rangle = A\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right)$$

$$\Delta E_1^{(2)} = \frac{|\langle 1|V'|0\rangle|^2}{\varepsilon_0 - \varepsilon_1} = A^2\frac{\hbar}{2m\omega}\cdot\frac{1}{\frac{1}{2}\hbar\omega - \frac{3}{2}\hbar\omega} = A^2\frac{\hbar}{2m\omega}\cdot\frac{1}{-\hbar\omega} = -\frac{A^2}{2m\omega^2}$$

$$\Delta E_2^{(2)} = \sum_{\substack{j\neq i\\ i=2}}\frac{|\langle j|V'|i\rangle|^2}{\varepsilon_i - \varepsilon_j} = \frac{|\langle 0|V'|1\rangle|^2}{\varepsilon_1 - \varepsilon_0} + \frac{|\langle 2|V'|1\rangle|^2}{\varepsilon_1 - \varepsilon_2} =$$

$$= A^2\frac{\hbar}{2m\omega}\,\frac{1}{\frac{3}{2}\hbar\omega - \frac{\hbar\omega}{2}} + A^2\frac{\hbar}{2m\omega}\,\frac{2}{\frac{3}{2}\hbar\omega - \frac{5\hbar\omega}{2}} =$$

$$= \frac{A^2\hbar}{2m\omega}\left[\frac{1}{\hbar\omega} + \frac{2}{-\hbar\omega}\right] = -\frac{A^2}{2m\omega^2}$$

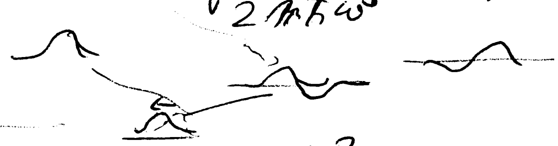
- 4th order gives zero
  ↳ see Wiki for equations

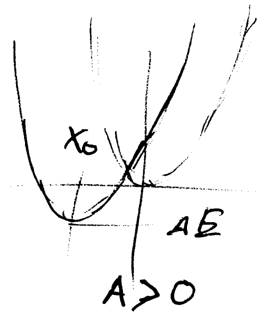
LHO + Ax only $j=1$ wavefunction

$$|\psi_0^{(1)}\rangle = |\psi_0\rangle + \sum_{j\neq 0} \frac{|j\rangle\langle j|V'|0\rangle}{\varepsilon_0-\varepsilon_j} =$$

$$= |0\rangle + A\sqrt{\frac{\hbar}{2m\omega}}\,\frac{1}{\frac{1}{2}\hbar\omega-\frac{3}{2}\hbar\omega}\,|1\rangle =$$

$$= |0\rangle - A\sqrt{\frac{1}{2m\hbar\omega^3}}\,|1\rangle$$





$$\left(\sqrt{\frac{m}{2}}\,\omega x + \frac{A}{\sqrt{2m}\,\omega}\right)^2 = \frac{m\omega^2}{2}\left(x+\frac{A}{m\omega^2}\right)^2$$

↳ $x-x_0$ → $x_0 = -\frac{A}{m\omega^2}$

center shifts into x_0

$$|0\rangle = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{\alpha}}\,e^{-\frac{x^2}{2\alpha^2}} \qquad \alpha=\sqrt{\frac{\hbar}{m\omega}}$$

$$|1\rangle = \frac{1}{\pi^{1/4}}\sqrt{\frac{2}{\alpha}}\,\frac{x}{\alpha}\,e^{-\frac{x^2}{2\alpha^2}}$$

$$|0\rangle = \frac{1}{\pi^{1/4}}\cdot\left(\frac{m\omega}{\hbar}\right)^{1/4} e^{-\frac{x^2}{2}\cdot\frac{m\omega}{\hbar}}$$

$$|1\rangle = \frac{1}{\pi^{1/4}}\sqrt{2}\cdot\left(\frac{m\omega}{\hbar}\right)^{1/4} x\cdot\sqrt{\frac{m\omega}{\hbar}}\,e^{-\frac{x^2}{2}\cdot\frac{m\omega}{\hbar}}$$

$$|0\rangle - A\cdot\sqrt{\frac{1}{2m\hbar\omega^3}}\,|1\rangle = \frac{1}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{1/4} e^{-\frac{x^2}{2}\cdot\frac{m\omega}{\hbar}}\left(1 - A\cdot\sqrt{\frac{1}{2m\hbar\omega^3}}\cdot\sqrt{2}\cdot x\cdot\sqrt{\frac{m\omega}{\hbar}}\right)$$

$$= \frac{1}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{1/4} e^{-\frac{x^2}{2}\left(\frac{m\omega}{\hbar}\right)}\cdot\left(1-\frac{A}{\hbar\omega}\cdot x\right) \neq \frac{1}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{1/4} e^{-\left(\frac{m\omega}{2\hbar}\right)\left(x+\frac{A}{m\omega^2}\right)^2}$$

op. posunutí $T(x_0) = 1 + x_0\frac{d\psi(x)}{dx} + \frac{x_0^2}{2}\frac{d^2\psi(x)}{dx^2} + \dots$

higher orders of perturb. theor. $\frac{A}{m\omega^2}$ -sums to exp...

→ 2^{nd} order sufficient to get the energy but ∞ order needed for wavefunction

LHO + $Axy + B(x^2+y^2)$

$$V' = A\frac{\alpha^2}{2}(a^+ + a)\otimes(b+b^+) + B\frac{\alpha^2}{2}(a^2+a^{+2}+2a^+a+1) +$$

$$B\frac{\alpha^2}{2}\,1\otimes(b^2+b^{+2}+2b^+b+1)$$

xy : $x\pm1 \wedge y\pm1$ $\quad x^2$: $x \begin{smallmatrix}+2\\0\\-2\end{smallmatrix}$ $y\to0$ $\quad y^2$: $x\to0$ $y\begin{smallmatrix}+2\\0\\-2\end{smallmatrix}$

1st PT ~~diag.~~ elements:

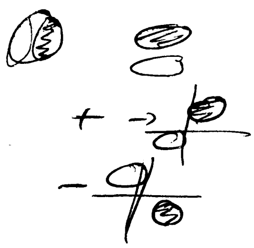
$\langle00|V'|00\rangle = \alpha^2B$

$\langle10|V'|10\rangle = 2\alpha^2B = \langle01|V'|01\rangle$

$$\langle10|V'|01\rangle = \langle10|A\frac{\alpha^2}{2}(a^+ + a)\otimes(b+b^+)|01\rangle =$$

$$= A\frac{\alpha^2}{2}\langle10|a^+\otimes b|01\rangle = A\frac{\alpha^2}{2}$$

$$\begin{vmatrix}2\alpha^2B & A\frac{\alpha^2}{2}\\ A\frac{\alpha^2}{2} & 2\alpha^2B\end{vmatrix} \to 2\hbar\omega + 2\alpha^2B \pm \frac{\alpha^2A}{2}$$



$\langle20|V'|20\rangle = \langle02|V'|02\rangle = \langle11|V'|11\rangle = 3\alpha^2B$

$\langle20|V'|02\rangle = 0$

$$\langle20|V'|11\rangle = \frac{A\alpha^2}{2}\langle20|\underset{\sqrt{2}}{(a^+ + a)}\otimes(b^+ + b)|11\rangle =$$

$$= \frac{A\alpha^2}{2}\sqrt{2}$$

$$\to 3\alpha^2B\begin{array}{c}|20\rangle\ |02\rangle\ |11\rangle\\ \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\end{array} + A\alpha^2\frac{\sqrt{2}}{2}\begin{pmatrix}0&0&1\\0&0&1\\1&1&0\end{pmatrix}$$

~~$\langle20|V'$~~

$$\begin{vmatrix}-\lambda & 0 & 1\\ 0 & -\lambda & 1\\ 1 & 1 & -\lambda\end{vmatrix} = -\lambda^3+2\lambda = -\lambda(\lambda^2-2) = -\lambda(\lambda+\sqrt{2})(\lambda-\sqrt{2})$$

$$\begin{pmatrix}-\sqrt{2} & 0 & 1\\ 0 & -\sqrt{2} & 1\\ 1 & 1 & -\sqrt{2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = 0$$

$-\sqrt{2}c_1 + c_3 = 0$

$-\sqrt{2}c_2 + c_3 = 0$

$c_1 + c_2 - \sqrt{2}c_3 = 0$

$c_1 = \frac{c_3}{\sqrt{2}}$

$c_1^2 + c_2^2 + c_3^2 = 1$

$\frac{c_3^2}{2} + \frac{c_3^2}{2} + c_3^2 = 1$

$2c_3^2 = 1$

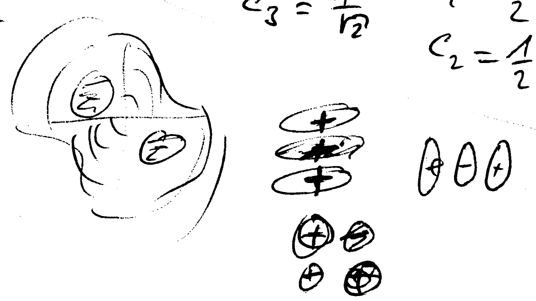
$c_3 = \frac{1}{\sqrt{2}}$ $\quad c_1 = \frac{1}{2}$

$c_2 = \frac{1}{2}$

$$\begin{pmatrix}\sqrt{2} & 0 & 1\\ 0 & \sqrt{2} & 1\\ 1 & 1 & \sqrt{2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = 0$$

$c_1 = \frac{1}{2}$ $\quad c_2 = \frac{1}{2}$

$c_3 = -\frac{1}{\sqrt{2}}$



$$\begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 1\\ 1 & 1 & 0\end{pmatrix}\begin{pmatrix}c_1\\c_2\\c_3\end{pmatrix} = 0$$

$c_1 = +\frac{1}{\sqrt{2}}$

$c_2 = -\frac{1}{\sqrt{2}}$

3D oscillator with $V' = Axy$ Lim 5051

? energies of first excited state?

$$x = \frac{\alpha}{\sqrt{2}}(a + a^+)$$

- states $|100\rangle$, $|010\rangle$, $|001\rangle$

$$V' = \frac{\alpha^2}{2}(a + a^+) \otimes (b + b^+) \otimes 1$$

$$\langle 100|V'|100\rangle = 0 \qquad = \langle 010|V'|010\rangle \qquad = \langle 001|V'|001\rangle$$

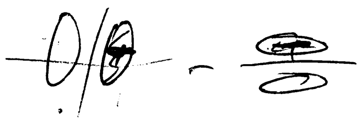
$\hookrightarrow x \to \pm 1$ and $y \pm 1$

$$\langle 100|V'|010\rangle = \frac{\alpha^2}{2}A\langle 100|(a+a^+)\otimes(b+b^+)\otimes 1|010\rangle$$

$$= \frac{\alpha^2}{2}A\langle 1|a^+|0\rangle_x \langle 0|b|1\rangle_y \langle 0|1|0\rangle_z = \frac{\alpha^2}{2}A$$

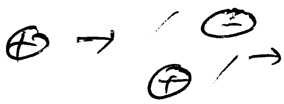
$$= \langle 010|V'|100\rangle$$

$$\to \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \to \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} = -\lambda^3 + \lambda = -\lambda(\lambda+1)(\lambda-1)$$

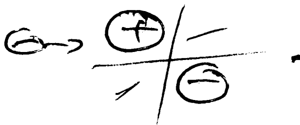


$\to \lambda_1 = 0$

$\lambda_{2,3} = \pm \frac{\alpha^2}{2}A$



$\to +\frac{\alpha^2}{2}A$



$-\frac{\alpha^2}{2}A$

$\frac{1}{\sqrt{2}}(|100\rangle + |010\rangle)$ $\qquad$ $\frac{1}{\sqrt{2}}(|100\rangle - |010\rangle)$

vs Ax^2y^2 LHO + Ax^2y^2 PChT-A.10

$$V' = A\cdot\frac{\alpha^4}{4}\left(a^2+a^{+2}+2a^+a+1\right)\otimes\left(b^2+b^{+2}+2b^+b+1\right)$$

- ~~jedná se~~ = 0 - pokud změna v jednom kanálu o jedna, tři, nebo nic, jinak ≠ 0

+2 +2
0 0
−2 −2

$$\langle 00|V'|00\rangle = A\cdot\frac{\alpha^4}{4}\langle 0_a|2a^+a+1|0_a\rangle\cdot\langle 0_b|2b^+b+1|0_b\rangle =$$

$$= A\cdot\frac{\alpha^4}{4}\cdot 1 = \frac{A\alpha^4}{4}$$

$|10\rangle, |01\rangle$ - nic, 1st order posuv, degenerace se nesnímá

$$\langle 20|V'|20\rangle = A\cdot\frac{\alpha^4}{4}\langle 2|\underbrace{2a^+a+1}_{2\cdot 2+1}|2\rangle\cdot\langle 0_b|\underbrace{2b^+b+1}_{1}|0_b\rangle$$

$|11\rangle$ - nic

$$= A\cdot\frac{\alpha^4}{4}\cdot 5 = \frac{5\alpha^4 A}{4}$$

$$\langle 20|V'|02\rangle = A\cdot\frac{\alpha^4}{4}\langle 2|a^{+2}|0\rangle\cdot\langle 0|b^2|2\rangle =$$

$$= \frac{\alpha^4 A}{4}\cdot\sqrt{2}\cdot\sqrt{2} = \frac{\alpha^4 A}{2}$$

$x = \frac{1}{4}$

$$\rightarrow \begin{array}{c|cc} & |20\rangle & |02\rangle \\ \hline \langle 20| & \frac{5\alpha^4A}{4} & \frac{\alpha^4A}{2} \\ \langle 02| & \frac{\alpha^4A}{2} & \frac{5\alpha^4A}{4} \end{array} \rightarrow \frac{5\alpha^4A}{4} \pm \frac{\alpha^4A}{2} \rightarrow \frac{7}{4}\alpha^4A, \quad \frac{3}{4}\alpha^4A$$