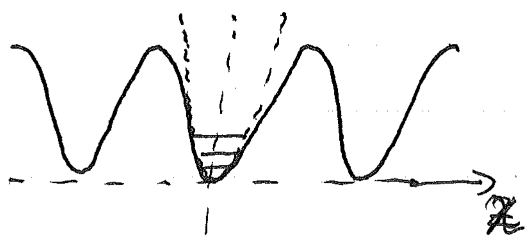
Lecture 12: Examples of Non-degenerate T.I.P.T.

- Optical Lattice: Trap for ultra-cold atoms ($T < 100\,\mu K$) created by interference pattern of intersecting laser beam. Trapping interaction = "ac-Stark shift" (see P.S. #1)

One dimensional example: standing wave

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{U}(x)$$

$$\hat{U}(x) = U_0 \sin^2 k_L x \qquad \text{where } k_L = \text{laser wave number}$$



Really periodic potential $\Rightarrow$ energy bands. But, for tight localization (near bottom of the well), we can ignore tunneling between lattice sites
$\Rightarrow$ Anharmonic oscillator

Near $x = 0$ $\quad \hat{U}(x) = U_0 \left(-k_L \hat{x} + \frac{1}{6} k_L^3 \hat{x}^3 + \dots\right)^2$

$$= \underbrace{(U_0 k_L^2)}_{\frac{1}{2} m\omega^2} \hat{x}^2 - \frac{U_0}{3} k_L^4 \hat{x}^4$$

Oscillation frequency $\quad \omega = \sqrt{2U_0 \frac{k_L^2}{m}} = \frac{2}{\hbar}\sqrt{U_0 E_R}$

$$E_R = \frac{(\hbar k_L)^2}{2m} \quad \text{"recoil energy"}$$

Thus, $$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2}_{\hat{H}_0} \underbrace{- \frac{U_0}{3}k_L^4\hat{x}^4}_{\hat{H}_1}$$

What is the small parameter? To find it, make $\hat{H}$ dimensionless (i.e. identify characteristic scales)

Recall for SHO, characteristic units: $\hat{X} \equiv \frac{\hat{x}}{x_c}$, $\hat{P} \equiv \frac{\hat{p}}{p_c}$

$$x_c = \sqrt{\frac{\hbar}{m\omega}}, \quad p_c = \sqrt{\hbar m\omega}, \quad E_c = \frac{p_c^2}{m} = m\omega^2 x_c^2 = \hbar\omega$$

$$\hat{h}_1 \equiv \frac{\hat{H}_1}{\hbar\omega} = -\frac{U_0}{3\hbar\omega}k_L^4\frac{\hbar^2}{m^2\omega^2}\hat{X}^4 = -\frac{E_R}{3\hbar\omega}\hat{X}^4$$

Small parameter $\lambda = \frac{E_R}{3\hbar\omega}$ $\Rightarrow$ (Require deep lattice so that zero point is near bottom)

First order perturbation corrections

$$E_n^{(0)} = \hbar\omega(n+\tfrac{1}{2}) \qquad |n^{(0)}\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0^{(0)}\rangle$$

$$\hat{X} = \frac{1}{\sqrt{2}}(\hat{a}+\hat{a}^\dagger)$$

$$E_n^{(1)} = \langle n^{(0)}|\hat{H}_1|n^{(0)}\rangle = -\frac{E_R}{3}\langle n^{(0)}|\hat{X}^4|n^{(0)}\rangle$$

Use operator algebra

(next page)

Aside: $\langle n^{(0)}| \hat{X}^4 | n^{(0)}\rangle = \frac{1}{4} \langle n^{(0)}| (\hat{a}+\hat{a}^\dagger)^4 | n^{(0)}\rangle$

$$\langle n^{(0)}| (\hat{a}+\hat{a}^\dagger)^4 | n^{(0)}\rangle = \langle n^{(0)}| (\hat{a}^2+\hat{a}^{\dagger 2}+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})^2 | n^{(0)}\rangle$$

$$= \langle n^{(0)}| (\hat{a}^2+\hat{a}^{\dagger 2}+2\hat{N}+1)^2 | n^{(0)}\rangle =$$ (keep only terms with equal # of $\hat{a}$ and $\hat{a}^\dagger$)

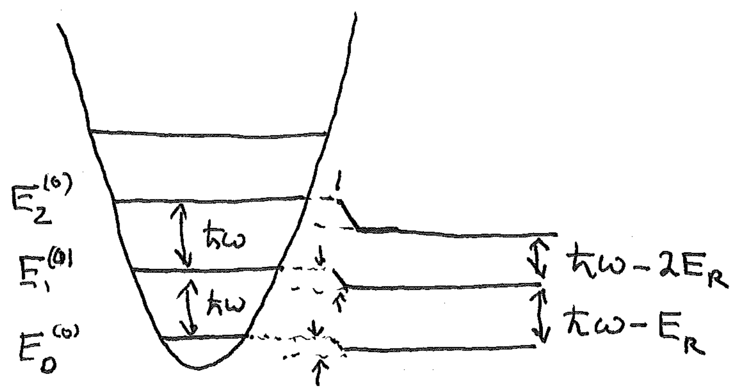
$$= \langle n^{(0)}| \left[\hat{a}^2\hat{a}^{\dagger 2}+\hat{a}^{\dagger 2}\hat{a}^2+(2\hat{N}+1)^2\right] | n^{(0)}\rangle$$

$$= \| \hat{a}^{\dagger 2} | n^{(0)}\rangle\|^2 + \| \hat{a}^2 | n^{(0)}\rangle\|^2 + (2n+1)^2$$

$$= (n+2)(n+1) + (n-1)n + (2n+1)^2$$

$$= 6\left(n^2+n+\tfrac{1}{2}\right)$$

$$\Longrightarrow \boxed{E_n^{(1)} = -\frac{E_R}{2}\left(n^2+n+\frac{1}{2}\right)}$$



Non-evenly spaced levels

Energy spacing in first order in $\frac{E_R}{\hbar\omega}$

$$\boxed{E_n - E_{n-1} = \hbar\omega - nE_R}$$

• Stark effect : Atom in a D.C. electric field
(consider hydrogen here)

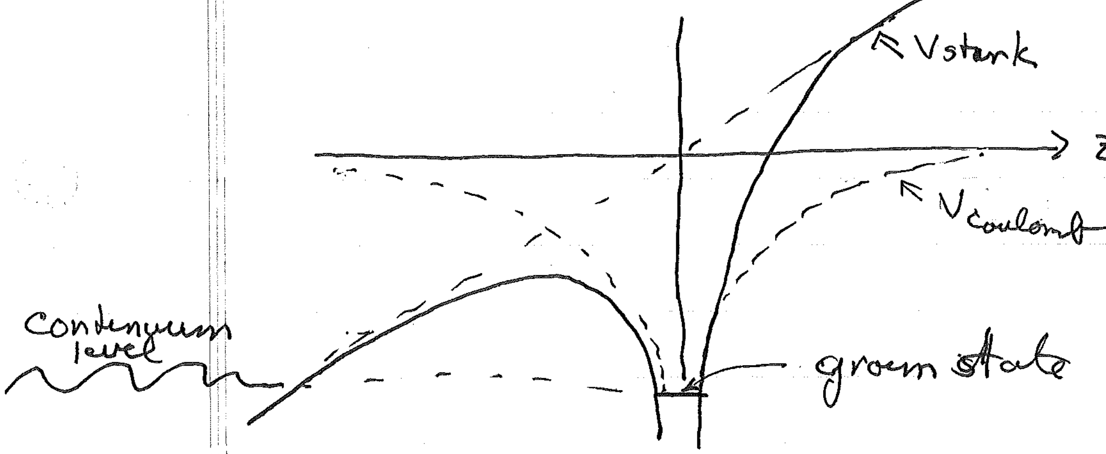
Force on electron $\vec{F} = -e\vec{\mathcal{E}}$

$\Rightarrow$ Interaction potential $\hat{V}_{int} = e\,\vec{\mathcal{E}} \cdot \hat{\vec{x}} = -\hat{\vec{d}} \cdot \vec{\mathcal{E}}$

$\hat{\vec{d}} = -e\hat{\vec{x}}$: electric dipole moment of electron (relative to the nucleus)

Total potential energy $\hat{V} = \frac{e}{r} - \hat{\vec{d}} \cdot \hat{\vec{\mathcal{E}}}$

Take $\vec{\mathcal{E}}$ is z-direction. Plot at $x = y = 0$



No matter how small $\vec{\mathcal{E}}$ is $\hat{V}_{int}$ diverges

$\Rightarrow$ Perturbation series diverges!

Reason: Coupling to continuum (tunneling)

However, tunnelling is <u>negligible</u> if $\vec{\mathcal{E}}$ is small enough

Recall: $\mathcal{E}_{internal} = \frac{e}{a_0} \simeq 10^9 \frac{\text{Volts}}{\text{cm}}$ $\Rightarrow$ Require $\mathcal{E} << \mathcal{E}_{internal}$

Given this caveat

Consider 1s state of hydrogen

$$E_{1s}^{(1)} = \langle 1s|\hat{V}_{int}|1s\rangle = e\vec{\mathcal{E}}\cdot\langle 1s|\hat{\vec{x}}|1s\rangle$$

Wavefunction of 1s state is spherically symmetric $\Longrightarrow$ $\langle 1s|\vec{x}|1s\rangle = 0$

More generally eigenstates $|n,l,m\rangle$ are parity eigenstates

$$\hat{\Pi}|n,l,m\rangle = (-1)^l|n,l,m\rangle$$

$\hat{\vec{x}}$ is odd under parity $\quad \hat{\Pi}^\dagger\hat{\vec{x}}\hat{\Pi} = -\hat{\vec{x}}$

$\Rightarrow$ Parity selection rule:

$$\langle n'l'm'|\hat{\vec{x}}|n\,l\,m\rangle = \langle n'l'm'|\hat{\Pi}^\dagger\underbrace{\hat{\Pi}\,\hat{\vec{x}}\,\hat{\Pi}^\dagger}_{-\hat{\vec{x}}}\hat{\Pi}|n\,l\,m\rangle$$

$$= -(-1)^{l+l'}\langle n'l'm'|\hat{\vec{x}}|n\,l\,m\rangle$$

$$\boxed{\text{selection rule: } \Delta l \text{ odd}}$$

$\Rightarrow$ ~~XXXX~~ First order correction vanishes

Go to second order

$$E_{1s}^{(2)} = \left[\sum_{n',l',m}\frac{|\langle n',l',m|z|1,0,0\rangle|^2}{E_{1s}^{(0)} - E_{n'l'}^{(0)}}\,e^2\right]\mathcal{E}_z^2$$

"Quadratic Stark shift" (second power of $|\vec{\mathcal{E}}|$)

[Unperturbed energy levels of Hydrogen

$$E_n^{(0)} = -\frac{e^2}{2a_0}\frac{1}{n^2}$$

$$\Rightarrow E_n^{(2)} = -2\, a_0\, \mathcal{E}_z^2 \sum_{n',l',m'} \frac{|\langle n' l' m' | \hat{z} | 1\,0\,0\rangle|^2}{\left(1 - \frac{1}{n'^2}\right)}$$

Aside: Recall $z = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1,0}(\theta)$, $Y_{00} = \frac{1}{\sqrt{4\pi}}$

$$\Rightarrow \langle n' l' m' | z | 1 0 0 \rangle = \int d\bar{r}\, u^*_{n'l'}\, \bar{r}\, u_{10} \int d\Omega\, Y^*_{l'm'} Y_{10} Y_{00}$$

$$\int d\Omega\, Y^*_{l'm'} Y_{10} Y_{00} = \frac{1}{\sqrt{4\pi}} \int d\Omega\, Y^*_{l'm'} Y_{10} = \frac{1}{\sqrt{4\pi}}\, \delta_{l',1}\, \delta_{m',0}$$

Selection rule: for $\vec{\mathcal{E}}$ along z $\boxed{\begin{array}{c}\Delta l = 1 \\ \Delta m = 0\end{array}}$

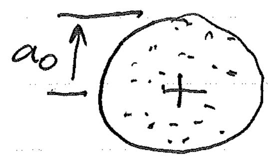
$$\Rightarrow E_n^{(2)} = -2\, a_0^3\, \mathcal{E}_z^2 \sum_{n'} \left[\frac{|d_{radial}(n')|^2}{1 - \frac{1}{n'^2}}\right]$$

where radial integral $d_{rad} = \frac{1}{\sqrt{3}} \int_0^\infty d\bar{r}\, \bar{r}\, u_{n1}(\bar{r})\, u_{10}(\bar{r})$

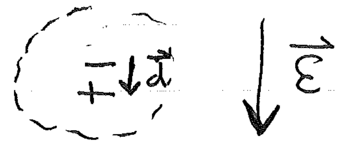
The sum can be done (see Bethe-Salpeter "One + Two electron atoms")

$$\boxed{\text{Result} \quad \Delta E_{1s}^{(2)} = -\frac{9}{4} a_0^3\, \mathcal{E}_z^2}$$

Physical picture: Induced dipole of polarizable particle



Unperturbed Hydrogen



Induced dipole interacts with $\vec{\mathcal{E}}$ (second order process)

Charge on spring picture

Balance restoring force

$$m\omega^2 z_{eq} = e\,\mathcal{E}_z$$

$$\Rightarrow \quad z_{eq} = \frac{e}{m\omega^2}\mathcal{E}_z$$

$\Rightarrow$ Induced dipole moment $\vec{d}_{ind} = \underbrace{\frac{e^2}{m\omega^2}}_{\alpha}\vec{\mathcal{E}}$

$$\alpha = \text{Polarizability} = \frac{e^2}{m\omega^2}$$

Total potential energy: $\frac{1}{2}m\omega^2 z_{eq}^2 - \vec{d}_{ind}\cdot\vec{\mathcal{E}}$

$$U = \frac{1}{2}m\omega^2\left(\frac{e}{m\omega^2}\mathcal{E}_z\right)^2 - \frac{e^2}{m\omega^2}\mathcal{E}_z^2$$

$$= -\frac{1}{2}\frac{e^2}{m\omega^2}\mathcal{E}_z^2 = \boxed{-\frac{1}{2}\alpha\,\mathcal{E}_z^2}$$

$$= -\frac{1}{2}\vec{d}_{ind}\cdot\vec{\mathcal{E}}$$

$\Uparrow$

half the potential is stored in "spring"

Quantum Mechanically

Induced dipole: $\langle \tilde{\phi} | \hat{\vec{d}} | \tilde{\phi} \rangle$ where

$$|\tilde{\phi}\rangle = \left(|\phi_{1s}^{(0)}\rangle + |\phi^{(1)}\rangle \right) / \|\tilde{\phi}\|$$

$$|\phi^{(0)}\rangle = |1s\rangle \qquad |\phi^{(1)}\rangle = e\mathcal{E}\sum_{n'} |n'10\rangle \frac{\langle n'10| \cancel{z} |100\rangle}{E_{1s} - E_{n'p}}$$

To lowest order: $$\langle \hat{\vec{d}} \rangle = \frac{\langle \phi_{1s}^{(0)} | \hat{\vec{d}} | \phi^{(1)} \rangle + \langle \phi^{(1)} | \hat{\vec{d}} | \phi^{(0)} \rangle}{1 + \cancel{\langle \phi^{(1)} | \phi^{(1)} \rangle} \to \text{neglect}}$$

$$\Rightarrow \langle \hat{\vec{d}} \rangle \equiv \vec{d}_{\text{induced}} = -2e^2 \sum_{n'} \frac{\langle 100 | \hat{z} | n'10 \rangle \langle n'10 | \hat{z} | n10 \rangle}{E_{1s} - E_{n'p}} \hat{\varepsilon}_z$$

$$\vec{d}_{ind} = \alpha \vec{\mathcal{E}} \Rightarrow \boxed{\alpha = +2e^2 \sum_{n'} \frac{\langle 100 | \hat{z} | n'10 \rangle \langle n'10 | \hat{z} | 100 \rangle}{E_{n'p} - E_{1s}}}$$

Polarizability (scalar here)

$$E_{1s}^{(2)} = -\frac{1}{2} \alpha \mathcal{E}^2 \quad \checkmark$$

Compare to classical picture:

Oscillator strength $$f_{nn'} \equiv \frac{|\langle n'10 | z | 100 \rangle|^2}{\left(\frac{\hbar}{2m\omega}\right)}$$

Majority of oscillator strength in the $1s \to 2p$ transition