5 Time Independent Perturbation (non-degen)

$H = H_0 + V$ — pertrb

H_0 ~ unpertrb

Given $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$

Desire to solve $(H_0+V)|n\rangle = E_n|n\rangle$

Customary to solve $(H_0+\lambda V)|n\rangle = E_n|n\rangle$ by intro. $\lambda \in [0,1]$ to indicate # of pertrb enters.

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ex two state sys.

Suppose $H = E_1^{(0)}|1^{(0)}\rangle\langle 1^{(0)}| + E_2^{(0)}|2^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{12}|1^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{21}|2^{(0)}\rangle\langle 1^{(0)}|$

ie $H = \begin{pmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{21} & E_2^{(0)} \end{pmatrix}$ let V_{12}, V_{21} real. by hermiticity $V_{12} = V_{21}$

Recall spin-orientation prob.

$$H_s = a_0 + \vec{\sigma}\cdot\underset{(a_1,0,a_3)}{\vec{a}} = \begin{pmatrix} a_0+a_3 & a_1 \\ a_1 & a_0-a_3 \end{pmatrix} \text{ has eigval. } E = a_0 \pm \sqrt{a_1^2+a_3^2}$$

By analogy, eigval of H

$$E_{1,2} = \frac{E_1^{(0)}+E_2^{(0)}}{2} \pm \sqrt{\frac{(E_1^{(0)}-E_2^{(0)})^2}{4} + \lambda^2|V_{12}|^2}$$

for $\lambda|V_{12}| \ll |E_1^{(0)}-E_2^{(0)}|$ binomial expansion yields

$$E_1 = E_1^{(0)} + \frac{\lambda^2|V_{12}|^2}{(E_1^{(0)}-E_2^{(0)})} + \cdots \qquad E_2 = E_2^{(0)} + \frac{\lambda^2|V_{12}|^2}{(E_2^{(0)}-E_1^{(0)})} + \cdots$$

w/ series converges $|V_{12}| < \left|\frac{E_1^{(0)}-E_2^{(0)}}{2}\right|$

Formal Construction.

$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$ $\{|n^{(0)}\rangle\}$ complete. and Pertrd sys. $(H_0+\lambda V)|n\rangle = E_n|n\rangle$ (*)

under pertrb, expect energy shift $\boxed{\Delta_n = E_n - E_n^{(0)}}$

Rewrite (*),

$$(E_n^{(0)} - H_0)|n\rangle = (\lambda V - \Delta_n)|n\rangle \qquad \text{principle eqn.}$$

note. $\frac{1}{E_n^{(0)}-H_0}$ singular if LHS acts on $|n\rangle \to |n^{(0)}\rangle$.

- $(\lambda V - \Delta_n)|n\rangle$ no $|n^{(0)}\rangle$ component ie $\langle n^{(0)}|(E_n^{(0)}-H_0)|n\rangle = 0$
- Def $\phi_n = \sum_{k\neq n}|k^{(0)}\rangle\langle k^{(0)}|$ then $\frac{1}{E_n^{(0)}-H_0}\phi_n = \sum_{k\neq n}\frac{1}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle\langle k^{(0)}|$ thus $(E_n^{(0)}-H_0)^{-1}$ well define
- also write $(\lambda V - \Delta_n)|n\rangle = \phi_n(\lambda V - \Delta_n)|n\rangle$ using completeness

so can now approximate $|n\rangle$ & $\Delta_n (E_n)$.

(A) $|n\rangle = C_n(\lambda)|n^{0}\rangle + \frac{1}{E_n^{(0)}-H_0}\phi_n(\lambda V - \Delta_n)|n\rangle$ w/ $\langle n^{(0)}|n\rangle = C_n(\lambda) = 1$

and

(B) $\Delta_n = \lambda\langle n^{(0)}|V|n\rangle$

Take $|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots$

$\Delta_n = \lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + \cdots$

Sub into (A) & (B)

then $O(\lambda)$ $\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$ $\quad |n^{(1)}\rangle = \frac{\phi_n}{E_n^{(0)}-H_0}V|n^{(0)}\rangle$

$O(\lambda^2)$ $\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle$ $\quad \Rightarrow \Delta_n^{(2)} = \langle n^{(0)}|\frac{V\phi_n V}{E_n^{(0)}-H_0}|n^{(0)}\rangle$

⋮

thus $\Delta_n = \lambda V_{nn} + \lambda^2 \sum_{k\neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} + \ldots$ w/ $V_{nk} = \langle n^{(0)} | V | k^{(0)} \rangle$

$$\boxed{\begin{array}{ll} 1^{st}\text{ order} & \Delta_n^{(1)} = V_{nn} = \langle n^{(0)} | V | n^{(0)} \rangle \\ 2^{nd}\text{ order} & \Delta_n^{(2)} = \sum_{k\neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} \end{array}}$$

$$|n\rangle = |n^{(0)}\rangle + \lambda \boxed{\sum_{k\neq n} \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle} + \lambda^2 \left(\sum_{k\neq n}\sum_{\ell\neq n} \frac{V_{k\ell} V_{\ell n} |k^{(0)}\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_\ell^{(0)})} - \sum_{k\neq n} \frac{V_{nn} V_{kn} |k^{(0)}\rangle}{(E_n^{(0)} - E_k^{(0)})^2} \right)$$

Renormalization

Def $|n\rangle_N = Z_N^{1/2} |n\rangle$ s.t. ${}_N\langle n | n\rangle_N = 1$ note $\langle n^{(0)} | n\rangle_N = Z_N^{1/2}$ — can find Z_N w/o knowing $|n\rangle_N$ first

thus ${}_N\langle n | n \rangle_N = Z_n \langle n | n \rangle = 1$

$$Z_n^{-1} = (\langle n^{(0)}| + \lambda \langle n^{(1)}| + \cdots) \times (|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \cdots) = 1 + \lambda^2 \langle n^{(1)} | n^{(1)}\rangle + O(\lambda^3)$$

$$= 1 + \lambda^2 \sum_{k\neq n} \frac{|V_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2} + O(\lambda^3)$$

$$Z_n \simeq 1 - \lambda^2 \underbrace{\sum_{k\neq n} \frac{|V_{kn}|^2}{(E_n^0 - E_k^0)^2}}_{\text{leakage}} < 1$$ note $\frac{1}{1-(-x)} \approx 1 + (-x) + \ldots$

From Δ_n, we also discover that

$$Z_n = \frac{\partial E_n}{\partial E_n^{(0)}}$$

ex SHO $H = \underbrace{\frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2}_{H_0} + \underbrace{\frac{1}{2} \varepsilon m \omega^2 x^2}_{V}$ note $\omega \to \sqrt{1+\varepsilon}\,\omega$

Recall. $|0\rangle = |0^{(0)}\rangle + \sum_{k\neq 0} \frac{V_{k0}}{E_0^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$ and $\Delta_0 = V_{00} + \sum_{k\neq 0} \frac{|V_{k0}|^2}{E_0^{(0)} - E_k^{(0)}} + \cdots$

$$V_{00} = \left(\frac{\varepsilon m \omega^2}{2}\right) \langle 0^{(0)} | x^2 | 0^{(0)}\rangle = \frac{\varepsilon \hbar\omega}{4} \qquad V_{20} = \left(\frac{\varepsilon m\omega^2}{2}\right) \langle 2^{(0)} | x^2 | 0^{(0)} \rangle = \frac{\varepsilon \hbar \omega}{2\sqrt{2}}$$

then $|0\rangle = |0^{(0)}\rangle - \frac{\varepsilon}{4\sqrt{2}} |2^{(0)}\rangle + O(\varepsilon^2)$

$$\Delta_0 = E_0 - E_0^{(0)} = \hbar\omega \left[\frac{\varepsilon}{4} - \frac{\varepsilon^2}{16} + O(\varepsilon^3) \right]$$

note
- $[H, \Pi] = 0$, $|n\rangle$ non-degen $|n\rangle$ parity ket
- $\underbrace{c_1 |0^{(0)}\rangle}_{\text{even}} + \underbrace{c_2 |1^{(0)}\rangle}_{\text{odd}}$ can't be parity ket

thus $|1^{(0)}\rangle$ component vanished.

Exact soln. $\frac{\hbar\omega}{2} \to \frac{\hbar\omega}{2}\sqrt{1+\varepsilon} = \frac{\hbar\omega}{2}\left(1 + \frac{\varepsilon}{2} - \frac{\varepsilon^2}{8} + \cdots\right)$

$$\langle x | 0^{(0)} \rangle = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{x_0}} e^{-x^2/2x_0^2}$$ where $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$ $\quad x_0 \to \frac{x_0}{(1+\varepsilon)^{1/4}}$

Hence,

$$\langle x | 0^{(0)} \rangle \simeq \langle x | 0^{(0)} \rangle - \frac{\varepsilon}{4\sqrt{2}} \langle x | 2^{(0)} \rangle \;!$$

ex quadratic stark effect

$H_0 = \frac{p^2}{2m} + V_0(r)$ and $V = -e|\vec{E}|z$

Ignored spin $\Rightarrow$ no degen energy level $|n\rangle$ are parity ket

$E_n = -\frac{Z^2 e^2}{2n^2 a_0}$ $\quad a_0 = \frac{\hbar^2}{m_e e^2}$ Bohr radius.

Consider ground state $n=1$ $l=m=0$, so energy shift

$$\Delta_k = E_k - E_k^{(0)} = -e|E|\langle k^{(0)}|z|k^{(0)}\rangle + e^2|E|^2 \sum_{j\neq k} \frac{|z_{kj}|^2}{E_k^0 - E_j^0} + \dots$$

Remark: • on z_{kk} by selection rule $\boxed{z_{kk}=0}$ (Recalled if $\varepsilon_\alpha \varepsilon_\beta \neq -1$ $\langle\beta|\vec{x}|\alpha\rangle = 0$) parity selection rule

• on z_{kj} $\boxed{\langle k|z|k\rangle \sim T_0^{(1)}}$ where $\langle n', l'm'|z|n, lm\rangle = 0$ unless $\begin{cases} l' = l\pm 1 \\ m' = m \end{cases}$

(By Wigner-Eckart thm: $\langle\alpha', j'm'|T_q^k|\alpha, jm\rangle$ $m'=m+q$ & $|j-k| \leq j' \leq j+k$)

• Check accuracy of approx.

Given polarizability α $\quad \Delta = -\frac{1}{2}\alpha|\vec{E}|^2$, ground state $|0^{(0)}\rangle = |1,0,0\rangle$ (n, l, m)

then
$$\alpha = -2e^2 \sum_{k\neq 0}^{\infty} \frac{|\langle k^{(0)}|z|100\rangle|^2}{E_0^0 - E_k^0}$$

$$\boxed{\text{first } \sum_{k\neq 0} |\langle k^0|z|100\rangle|^2 = \sum_{\text{all } k} |\langle k^0|z|1,00\rangle|^2 = \sum \langle 100|z|k^0\rangle\langle k^0|z|100\rangle = \langle 100|z^2|100\rangle}$$

since $\langle z^2\rangle = \langle x^2\rangle = \langle y^2\rangle = \frac{1}{3}\langle r^2\rangle$ and $\langle r^2\rangle = a_0^2$

assume $E_0^0 - E_k^0 \sim$ constant

knowing $-E_0^0 + E_k^0 \geq -E_0^0 + E_1^0 = \frac{e^2}{2a_0}\left(1 - \frac{1}{4}\right)$ after some calculation

we have $\alpha < \frac{16a_0^3}{3} \simeq 5.3\, a_0^3$ where measured value $\alpha = \frac{9a_0^3}{2} = 4.5a_0^3$.

(~~non~~-degen) Intro

note $\frac{V_{nk}}{E_n^0 - E_k^0}$ singular if $V_{nk} \neq 0$ but denominator $= 0$

Now when degen, one is free to pick basis (unpertrb ket) s.t if $E_n^0 - E_k^0 = 0$, $V_{nk} = 0$

Assume g-fold degen b/f pertrb "V". i.e E_0^0 for g diff. $|m^0\rangle$.

then in general, pertrb V remove degen by adding g-pertrb kets $\{|l\rangle\}$ w/ diff. energy.

As $\lambda \to 0$ $|l\rangle \to |l^0\rangle$ various ket of H_0 w/ same E_m^0

$|l^0\rangle \neq |m^0\rangle$ in general

thus $|l^0\rangle = \sum_{m\in D} |m^0\rangle\langle m^0|l^0\rangle$

To simplify calculation (expansion)

Def P_0 proj. op. onto space of $\{|m^0\rangle\}$ and $P_1 = 1 - P_0$ onto remaining space.

Then SE:
$$0 = (E - H_0 - \lambda V)|l\rangle$$
$$= (E - H_0 - \lambda V)P_0|l\rangle + (E - H_0 - \lambda V)P_1|l\rangle$$
$$= (E - E_D^0 - \lambda V)P_0|l\rangle + (E - H_0 - \lambda V)P_1|l\rangle \quad (*)$$

note $P_0P_1 = 0$ $P_1^2 = P_1$ $P_0^2 = P_0$ $[H, P_{1,0}] = 0$

Applying P_0, P_1 on left of $(*)$,

(A) $P_0(E - E_D^0 - \lambda V)P_0|l\rangle - \lambda P_0 V P_1|l\rangle = 0$

(B) $-\lambda P_1 V P_0|l\rangle + P_1(E_0 - H_0 - \lambda V)P_1|l\rangle = 0$

Remark $P_1(E - H_0 - \lambda P_1 V P_1)$ not singular b/c $E \sim E_D^0$

using $P_1^2 = P_1$ we rewrite/express

$$P_1|l\rangle = P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 |l\rangle \quad \text{for } |l\rangle = |l^0\rangle + \lambda|l'\rangle + \cdots \quad P_1|l'\rangle = \sum_{k \neq D} \frac{|k^0\rangle V_{kl}}{E_D^0 - E_k^0}$$

By sub $P_1|l'\rangle$ into (A) for $P_0|l\rangle$:

$$\left(E - E_D^0 - \lambda P_0 V P_0 - \lambda^2 P_0 V P_1 \frac{1}{E - H_0 - \lambda V} P_1 V P_0\right) P_0|l\rangle = 0$$

using $|l\rangle = |l^0\rangle + \lambda|l'\rangle$ and $P_0|l\rangle \to P_0|l^0\rangle$

w/ order λ term where $\lambda^2 \ll 1$,

we have
$$(E - E_D^0 - \lambda P_0 V P_0)(P_0|l^0\rangle) = 0 \quad \text{"secular Eqn"}$$

this reduces to eigval problem of the $g \times g$ matrix $P_0 V P_0$

As $\lambda \to 1$, $\det(V - \underbrace{(E - E_D^0)}_{\Delta})$

w/ matrix elem. $\langle m^{(0)}|V|m'^{(0)}\rangle$ we recast secular Eqn:

$$\begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & V_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle 1^0|l^0\rangle \\ \langle 2^0|l^0\rangle \\ \vdots \end{pmatrix} = \Delta_l^{(1)} \begin{pmatrix} \langle 1^0|l^0\rangle \\ \langle 2^0|l^0\rangle \\ \vdots \end{pmatrix}$$

$\underline{ex}$ linear Stark Effect. $V = -ez|E|$

$E_n = \frac{-Z^2e^2}{2n^2a_0}$ $\quad Z=1$ here $\quad E_2 = -\frac{e^2}{8a_0}$

$n=2 \quad \ell=0 \quad \ell=1\ (m=\pm1,0)$

$\qquad\ \ 2s \qquad 2p$

$\langle n,\ell,m|V|n,\ell',m'\rangle$

- non-vanished element only between states of opp. parity ie. $\ell=0$ and $\ell=1$
  note that $z \sim T_0^{(1)}$ thus $\ell'=\ell\pm1$ and $m'=m$ for nonzero entries.
- matrix

$$\begin{array}{c|cccc} & 2s & 2P_{m=0} & 2P_{m=1} & 2P_{m=-1} \\ \hline 2s & & & & \\ 2P_{m=0} & & & & \\ 2P_{m=1} & & & & \\ 2P_{m=-1} & & & & \end{array}$$

$$\begin{array}{c} 2s \\ 2P_{m=0} \\ 2P_{m=1} \\ 2P_{m=-1} \end{array} \begin{pmatrix} 0 & \langle 2s|V|2P,m=0\rangle & 0 & 0 \\ \langle 2P,m=0|V|2s\rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

now $\langle 2s|V|2P,m=0\rangle = -e|\vec{E}|\langle 2s|z|2P,m=0\rangle = 3ea_0|\vec{E}|$

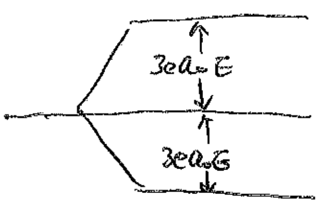
consider $\langle 200|z|210\rangle$

$$\left.\begin{array}{l} R_{20}(r) = \left(\frac{1}{2a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0} \\ R_{21}(r) = \left(\frac{1}{2a_0}\right)^{3/2}\frac{r}{\sqrt{3}\,a_0}e^{-r/2a_0} \end{array}\right\} \text{ then } \langle 200|z|210\rangle = 3a_0$$

so $\quad V = \begin{array}{c} \quad 2s \qquad 2P,m=0 \\ \begin{pmatrix} 0 & 3ea_0|E| \\ 3ea_0|E| & 0 \end{pmatrix} \end{array} \Rightarrow \Delta'_\pm = \pm 3ea_0|E|$

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|2s,m=0\rangle \pm |2P,m=0\rangle\right)$$

$$\Delta_\ell^{(1)} = \langle \ell^{(0)}|V|\ell^{(0)}\rangle \Rightarrow \Delta'_\pm = \langle \pm|V|\pm\rangle$$



$\frac{|2s,m=0\rangle - |2P,m=0\rangle}{\sqrt{2}}$

$|2P,m=\pm1\rangle$ no change

$\frac{|2s,m=0\rangle + |2P,m=0\rangle}{\sqrt{2}}$

$\underline{ex}$ Relativistic Correction to Kinetic Energy

$H_0 = \frac{\vec{p}^2}{2m_e} - \frac{Ze^2}{r}$ $\quad$ where $K = \sqrt{p^2c^2 + m_e^2c^4} - m_ec^2 \approx m_ec^2\left(1 + \frac{p^2}{2m_e^2c^2} - \frac{p^4}{8m_e^4c^4}\right)$

$$\therefore K = \frac{p^2}{2m_e} - \frac{p^4}{8m_e^3c^2}$$

thus $V = -\frac{(p^2)^2}{8m_e^3c^2}$

since $[\vec{L}, V] = 0$ we have $|n\ell m\rangle$

thus,

$$\Delta_{n\ell}^{(1)} = \langle n\ell m|V|n\ell m\rangle = \langle n\ell m| -\frac{(p^2)^2}{8m_e^3c^2}|n\ell m\rangle$$

ex spin-orbit interaction

$V_c(r) = e\phi(r)$ thus $\vec{E} = -\frac{1}{e}\nabla V_c(r)$

$\vec{B} = -\frac{\vec{v}}{c}\times\vec{E}$ w/ $\vec{\mu} = \frac{e\vec{S}}{m_e c}$

thus

$$H_{LS} = -\vec{\mu}\cdot\vec{B} = \vec{\mu}\cdot\left(\frac{\vec{v}}{c}\times\vec{E}\right) = \left(\frac{e\vec{S}}{m_e c}\right)\cdot\left[\frac{\vec{p}}{m_e c}\times\left(\frac{\vec{x}}{r}\right)\frac{1}{(-e)}\frac{dV_c}{dr}\right]$$

$$= \frac{1}{m_e^2 c^2}\frac{1}{r}\frac{dV_c}{dr}\left(\vec{L}\cdot\vec{S}\right)$$