# The Variational Method

$H|\varphi_n\rangle = E_n|\varphi_n\rangle$ $\qquad E_n, |\varphi_n\rangle$ unknown

arbitrary ket $\quad |\psi\rangle = \sum_n c_n|\varphi_n\rangle \; ; \quad \langle\psi|\psi\rangle = \sum_n |c_n|^2 = 1$

$$\langle\psi|H|\psi\rangle = \sum_n c_n^* \langle\varphi_n| E_n c_n |\varphi_n\rangle$$

$$= \sum_n |c_n|^2 E_n$$ e.g. expectation value

<u>Key Point</u>: I can always claim

$$\sum_n |c_n|^2 E_n \geq E_0 \sum_n |c_n|^2$$

because $E_0$ is the smallest energy (ground state).

We have equality only if $|\psi\rangle = |\varphi_0\rangle$

$$\Longrightarrow \langle H\rangle = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq \frac{E_0 \sum_n |c_n|^2}{\sum_n |c_n|^2} = E_0$$

So $\boxed{\langle H\rangle \geq E_0 \text{ always}}$

1) choose trial wavefunction

$|\psi(\alpha)\rangle$ → Ritz parameter

trial ket

which is "well-behaved" $\psi(x \to \pm\infty) = 0$

smooth enough

2) $\langle H \rangle (\alpha)$

3) minimize $\langle H \rangle (\alpha)$ w.r.t. $\alpha$

This will give an approximation to the energy ground state.

This allows you to estimate an upper bound on the ground state energy.

Ex: H.O. $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$

(a) $\psi_\alpha(x) = e^{-\alpha x^2}$ $\alpha > 0$

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = \int_{-\infty}^{\infty} e^{-\alpha x^2}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right] e^{-\alpha x^2}\, dx$$

Don't forget normalization

$$\langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2\alpha}}$$

$$\Longrightarrow \quad \frac{\langle \psi_\alpha | H | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} = \underbrace{\frac{\hbar^2 \alpha}{2m} + \frac{m\omega^2}{8\alpha}}_{\text{"mean as a function of } \alpha\text{"}}$$

$$\frac{\partial}{\partial \alpha} \langle H \rangle = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} = 0$$

$$\longrightarrow \quad \boxed{\alpha_0 = \frac{m\omega}{2\hbar}}$$

$$\longrightarrow \quad \langle H \rangle (\alpha_0) = \frac{\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{m\omega^2}{8}\frac{2\hbar}{m\omega}$$

$$= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \boxed{\frac{\hbar\omega}{2}}$$

This exact for H.O.

So we have found $E_0 \approx \hbar\omega/2$ which, in fact, is <u>exactly</u> the g.s. energy.

Same problem w/ crazy trial function

$$\psi_\alpha(x) = \frac{1}{x^2+\alpha} \quad , \qquad \alpha > 0$$

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = \int_{-\infty}^{\infty} \frac{1}{x^2+\alpha}\left( -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \right)\frac{1}{x^2+\alpha}\, dx$$

$$= \frac{\hbar^2}{8m}\frac{\pi}{\alpha^{5/2}} + \frac{m\omega^2\pi}{4\sqrt{\alpha}}$$

$$\langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{\infty} \frac{1}{(x^2+\alpha)^2}\, dx = \frac{\pi}{2\alpha\sqrt{\alpha}}$$

$$\Longrightarrow \quad \langle H \rangle(\alpha) = \frac{\hbar^2}{4m\alpha} + \frac{m\omega^2\alpha}{2}$$

$$\longrightarrow \quad \frac{\partial}{\partial\alpha}\langle H \rangle = -\frac{\hbar^2}{4m\alpha^2} + \frac{m\omega^2}{2} \Rightarrow \alpha_0 = \frac{\hbar}{\sqrt{2}m\omega}$$

$$\longrightarrow \quad \boxed{E_{gs} \approx \frac{\sqrt{2}}{2}\hbar\omega}$$

# Time Dependent Potentials

## The interaction picture

| Schrodinger | Heisenberg |
|---|---|
| $\|\alpha, t_0, t\rangle_S = \hat{U}(t_0 t)\,\|\alpha\, t_0\rangle$ | $\|\alpha, t_0; t\rangle_H = \|\alpha, t_0\rangle$ |
| propogator | $A_H(t) = \hat{U}^{+}(t, t_0)\, A_S\, \hat{U}(t, t_0)$ |

where $\hat{U}(t\ t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ for $H \neq H(t)$

Time evolution

| | |
|---|---|
| $H\|\psi\rangle = i\hbar\frac{\partial}{\partial t}\|\psi\rangle$ | $\frac{dA_H(t)}{dt} = \frac{1}{i\hbar}[A_H, H]$ |

Now we introduce a new picture:

Dirac (interaction) picture

useful for.

$$H = H_0 + V(t)$$

$$|\alpha, t_0; t\rangle_I = e^{-\frac{i}{\hbar}H(t-t_0)} |\alpha, t_0; t\rangle_S$$

$$|\alpha, t_0; t_0\rangle_I = |\alpha, t_0; t_0\rangle_S \qquad \underline{\underline{t_0 = 0}}$$

$$A_I = e^{\frac{iH_0 t}{\hbar}} A_S e^{-\frac{i}{\hbar}H_0 t}$$

$$\frac{dA_I}{dt} = \frac{1}{i\hbar}[A_I, H_0]$$

$$i\hbar \frac{\partial}{\partial t}|\alpha t_0; t\rangle_I = i\hbar \frac{\partial}{\partial t}\left(e^{\frac{i}{\hbar}H_0 t_0}|\alpha, t_0; t\rangle_S\right)$$

$$= -H_0 e^{\frac{i}{\hbar}H_0 t}|\alpha, t_0; t\rangle_S + e^{\frac{i}{\hbar}H_0 t} \underbrace{i\hbar\frac{\partial}{\partial t}|\alpha t_0; t\rangle_S}_{\text{use Schrödinger}}$$

$$= -H_0 e^{\frac{i}{\hbar}H_0 t}|\alpha, t_0; t\rangle_S + e^{\frac{i}{\hbar}H_0 t}(H_0 + V(t))|\alpha t_0; t\rangle_S$$

$$= V(t)\, e^{\frac{i}{\hbar}H_0 t}|\alpha t_0; t\rangle_S$$

$$\longrightarrow \quad \boxed{i\hbar\frac{\partial}{\partial t}|\alpha t_0; t\rangle_I = V_I |\alpha t_0; t\rangle_I}$$

# Time dependent potentials

Recall: $H_s = H_0 + V_s(t)$

Schrödinger's Equation

$$i\hbar \frac{\partial}{\partial t}|\alpha\, t_0; t\rangle = H_s |\alpha\, t_0; t\rangle \Rightarrow |\alpha\, t_0; t\rangle_I = e^{\frac{i}{\hbar}H_0 t}|\alpha\, t_0; t\rangle$$

$$V_I = e^{\frac{i}{\hbar}H_0 t} V_s e^{-i/\hbar H_0 t} \Rightarrow \boxed{i\hbar \frac{\partial}{\partial t}|\alpha\, t_0; t\rangle = V_I |\alpha\, t_0; t\rangle_I}$$

# Dirac Picture & time dependent potentials

"Interaction Picture"

both the state and operators are time dependent

Let's take this a little further

$H_0|n\rangle = E_n|n\rangle$ (given)

initial state $|i\rangle \xrightarrow{H = H_0 + V(t)} |f\rangle$ final state

$|\alpha\, t_0; t\rangle_I = \sum_n c_n(t)|n\rangle$ time dependence is in the coeffecients

if $|f\rangle = |\alpha\, t_0, t\rangle = \sum_n c_n(t)|n\rangle$

then $\longrightarrow P(|f\rangle) = \sum_n |c_n(t)|^2$

bracket w/ $\langle n|$

$$\langle n| \left( i\hbar \frac{\partial}{\partial t} |\alpha\, t_0\, t\rangle \right) = \langle n| \left( V_I \, |\alpha\, t_0\, t\rangle \right)$$

$$i\cancel{\hbar \tfrac{\partial}{\partial t}} \qquad i\hbar \frac{\partial}{\partial t} \underbrace{\langle n|\alpha\, t_0\, t\rangle}_{c_n(t)} = \sum_m \underbrace{\langle n|V_I|m\rangle}_{\text{matrix elem}} \underbrace{\langle m|\alpha\, t_0\, t\rangle}_{c_m(t)}$$

$$\langle n|V_I|m\rangle = \langle n| e^{\frac{i}{\hbar}H_0 t} \, V_S(t) \, e^{-\frac{i}{\hbar}H_0 t} |n\rangle$$

$$= e^{\frac{i}{\hbar}(E_n - E_m)t} \langle n| V_m(t) |m\rangle$$

$$= e^{\frac{i}{\hbar}(E_n - E_m)t} \, V_{nm}$$

back into original equation gives

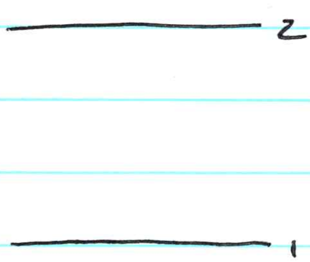
$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m V_{nm} e^{i\omega_{nm} t} c_m(t)$$

"coupled differential equations"

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & \cdots \\ V_{21}e^{i\omega_{21}t} & V_{22} & \\ \vdots & & V_{33} \\ & & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

How do we solve if $n$ runs to infinity?

Consider a 2 level system



$$H_0|n\rangle = E_n|n\rangle \qquad n=1,2$$

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$$

$$\doteq \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

apply time dependent field

$$V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1|$$

$$\gamma, \omega \in \mathbb{R}$$

@ $t=0$ only level 1 is populated

$$\longrightarrow \begin{cases} i\hbar \frac{\partial}{\partial t} c_1(t) = \gamma e^{i(\omega+\omega_{12})t} c_2(t) \\ i\hbar \frac{\partial}{\partial t} c_2(t) = \gamma e^{i(\omega-\omega_{12})t} c_1(t) \\ \\ c_1(0) = 1 \qquad c_2(0) = 0 \end{cases}$$

Methods to solve: go to second derivative

$$i\hbar \ddot{c}_1 = \underbrace{i(\omega+\omega_{12})\gamma e^{i(\omega+\omega_{12})t} c_2}_{i\hbar \frac{dc_1}{dt}} + \gamma e^{i(\omega+\omega_{12})t} \dot{c}_2$$

$$\frac{1}{i\hbar}\gamma e^{i(\omega+\omega_{12})t} c_1(t$$

$$\longrightarrow \quad \ddot{c}_1 - i(\omega+\omega_{12})\dot{c}_1 + \overbrace{\cancel{\quad}}^{\frac{\gamma^2}{\hbar^2}} c_1 = 0$$

$$\ddot{c}_2 + i(\omega+\omega_{12})\dot{c}_2 + \frac{\gamma^2}{\hbar^2} c_2 = 0$$

damped oscillator!

$$|c_2(t)|^2 = \frac{\gamma^2/\hbar^2}{\frac{\gamma^2}{\hbar^2}+(\omega+\omega_{12})^2/4} \sin^2\left(\sqrt{\frac{\gamma^2}{\hbar^2}+\frac{(\omega+\omega_{12})^2}{4}}\, t\right)$$

$$|c_1(t)|^2 = \quad '' \quad \cos^2( \quad '' \quad )$$

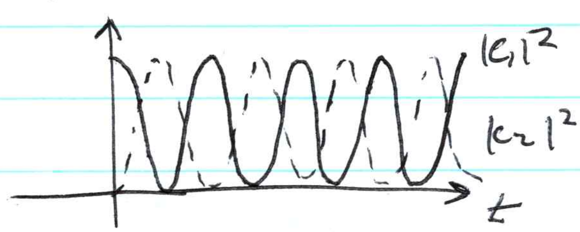
because $|c_1|^2 + |c_2|^2 = 1$ always

$$\boxed{\Omega \equiv \sqrt{\frac{\gamma^2}{\hbar^2}+\frac{(\omega+\omega_{12})^2}{4}}}$$ Rabi frequency!

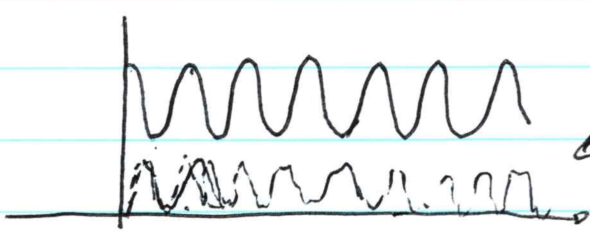
if $\omega+\omega_{12}=0 \Longrightarrow$ Resonance!

What happens when you are on Resonance?

$$\Omega_{res} = \frac{\gamma}{\hbar}$$




Off resonance:



still sum to 1 but

# What do we do if we have more than 2 levels?

## TIME DEPENDENT PERTURBATION THEORY

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$H_0|n\rangle = E_n|n\rangle$ ; $H = H_0 + V(t)$ $\qquad |i\rangle \xrightarrow{?} |f\rangle$

$$i\hbar \frac{d}{dt} C_n(t) = \lambda \sum_k V_{nk}(t) e^{i\omega_{nk}t} C_k(t)$$

to keep track of order of expansions.

Let $C_n(t) = C_n^0(t) + \lambda C_n^1(t) + \lambda^2 C_n^2(t) + \ldots$

$\lambda^0$: $i\hbar \dot{C}_n^0(t) = 0$ (potential already has $\lambda$)

$\hookrightarrow$ $C_n^0 = \delta_{ni}$ initial condition

$\lambda^1$: $i\hbar \dot{C}_n^1(t) = \sum_k V_{nk}(t) e^{i\omega_{nk}t} \overbrace{C_k^0}^{\delta_{ki}} = V_{ni} e^{i\omega_{ni}t}$

$\vdots$

$\lambda^r$: $i\hbar \dot{C}_n^{(r)}(t) = \sum_k V_{nk}(t) e^{i\omega_{nk}t} C_k^{(r-1)}$

$$\boxed{C_n^{(1)}(t) = \frac{1}{i\hbar}\int_0^t V_{ni}(t') e^{i\omega_{fi}t'} dt'}$$