The Variational Method

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

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

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

$$= \sum_n |c_n|^2 E_n$$ 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. α

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

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

$$\Longrightarrow \quad \frac{\langle \psi_\alpha | H | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} = \underbrace{\frac{\hbar^2 \alpha}{2m} + \frac{m\omega^2}{8\alpha}}$$

"mean as a function of α"

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

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

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

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

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

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

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

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

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

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

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

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

Time Dependent Potentials

The interaction picture

Schrodinger	Heisenberg
$\lvert \alpha, t_0, t \rangle_S = \hat{U}(t_0 t) \lvert \alpha\, t_0 \rangle$	$\lvert \alpha, t_0 ; t \rangle_H = \lvert \alpha, t_0 \rangle$
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

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

Now we introduce a new picture:

Dirac (interaction) picture

useful for.

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

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

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

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

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

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

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

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

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

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