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Relation between sol'ns of 2 particle and 1 particle Sch. Eqn

1 particle Schroedinger Eqn

(1) $$\left\{-\frac{\hbar^2}{2m}\nabla_1^2 + V(r_1)\right\}\psi_n(r_1) = E_n\psi_n(r_1)$$

2 particle Schroedinger Eqn

(2) $$\left\{-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(r_1) + V(r_2) + U(r_1 r_2)\right\}\tilde{\psi}_a(r_1 r_2) = \tilde{E}_a\tilde{\psi}_a(r_1 r_2)$$

If $U(r_1 r_2) = \phi$ can easily see

(3) $$\tilde{\psi}_a(r_1 r_2) = \psi_n(r_1)\psi_m(r_2)$$

Is soln of (2) with $\tilde{E}_a = E_n + E_m$.

But (3) violates antisymmetry requirement

(4) $$\tilde{\psi}_a(r_1 r_2) = -\tilde{\psi}_a(r_2 r_1)$$

Slight change works

(5) $$\tilde{\psi}_a(r_1 r_2) = \psi_n(r_1)\psi_m(r_2) - \psi_n(r_2)\psi_m(r_1)$$

Note this can be written $\begin{vmatrix} \psi_n(r_1) & \psi_m(r_1) \\ \psi_n(r_2) & \psi_m(r_2) \end{vmatrix}$

determinant

This obeys Antisymmetry requirement and also Pauli principle $\tilde{\psi}_\alpha(r_1 r_1) = \phi$.

Generalization to 3 particle Sch Eqn

$$\tilde{\psi}(r_1 r_2 r_3) = \begin{vmatrix} \psi_n(r_1) & \psi_m(r_1) & \psi_e(r_1) \\ \psi_n(r_2) & \psi_m(r_2) & \psi_e(r_2) \\ \psi_n(r_3) & \psi_m(r_3) & \psi_e(r_3) \end{vmatrix}$$

"Slater Determinant"

For example, note Pauli and antisymmetry okay

$\tilde{\psi}(r_1\ r_2\ r_1) = \phi$ because rows 1 + 3 of matrix identical → determinant vanishes

$\tilde{\psi}(r_1\ r_3\ r_2) = -\tilde{\psi}(r_1\ r_2\ r_3)$ because rows 2, 3 of determinant interchanged → determinant changes sign

Can do very little without a computer in the case $u(r_1, r_2) \neq 0$. But a pretty good approximation is

$$\tilde{\psi}(r_1 r_2) = e^{-\lambda u(r_1 r_2)} \begin{vmatrix} \psi_n(r_1) & \psi_m(r_1) \\ \psi_n(r_2) & \psi_m(r_2) \end{vmatrix}$$

Jastrow factor

Then minimize $\langle \hat{H} \rangle$ with respect to λ.

Variational Wave functions for single particle Sch. Eqn

① Guess form for wave function with 1 or more free parameters.

② Normalize it

③ Compute $\langle \psi | H | \psi \rangle$

④ Minimize with respect to free parameters

Example: δ function potential

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \alpha \delta(x) \right] \psi(x) = -|E| \psi(x)$$

Recall Exact soln. For $x \neq 0$ $\delta(x) = 0$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = -|E| \psi(x)$$

$$\Rightarrow \quad \psi(x) = e^{-\beta x} \quad \text{with} \quad \frac{\hbar^2 \beta^2}{2m} = |E|$$
$(x > 0)$

$$= e^{+\beta x}$$
$(x < 0)$

V-2

Integrate near origin

$$\int_{-\epsilon}^{\epsilon}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-\alpha\right]\psi(x) = \int_{-\epsilon}^{\epsilon}-|E|\psi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{x=\epsilon}-\left.\frac{d\psi}{dx}\right|_{x=-\epsilon}\right)-\alpha\psi(0) = \phi \text{ as } \epsilon\to 0$$

$$-\frac{\hbar^2}{2m}\left(-\beta-(\beta)\right)-\alpha=0$$

$$\beta=\frac{m\alpha}{\hbar^2}$$

$$|E|=\frac{\hbar^2\beta^2}{2m}=\frac{\hbar^2}{2m}\left(\frac{m}{\hbar^2}\right)^2\alpha^2$$

$$|E|=\frac{m\alpha^2}{2\hbar^2} \leftarrow \text{Exact}$$

Now try <u>variational</u>

V-3

(1) Make wrong guess $\psi(x) = n e^{-\lambda x^2/2}$

(2) Normalize $1 = \int |\psi(x)|^2 dx = n^2 \sqrt{\frac{\pi}{\lambda}}$

so $n = (\lambda/\pi)^{1/4}$

$$\psi(x) = (\lambda/\pi)^{1/4} e^{-\lambda x^2/2}$$

(3) Compute $\langle \psi | H | \psi \rangle$

$$= \left(\frac{\lambda}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\lambda x^2/2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x) \right) e^{-\lambda x^2/2}$$

$$= \left(\frac{\lambda}{\pi}\right)^{1/2} \left\{ \int e^{-\lambda x^2/2} \left[\left(-\frac{\hbar^2}{2m}\frac{d}{dx} \right) \left(-\lambda x e^{-\lambda x^2/2} \right) \right] dx - \alpha \right\}$$

$$= \left(\frac{\lambda}{\pi}\right)^{1/2} \left\{ \int \frac{\hbar^2 \lambda}{2m} \underbrace{e^{-\lambda x^2} dx}_{\sqrt{\frac{\pi}{\lambda}}} - \int \frac{\hbar^2 \lambda^2}{2m} \underbrace{x^2 e^{-\lambda x^2} dx}_{\frac{1}{2\lambda}\sqrt{\frac{\pi}{\lambda}}} - \alpha \right\}$$

$$= \left(\frac{\lambda}{\pi}\right)^{1/2} \left\{ \frac{1}{2} \frac{\hbar^2}{2m} \lambda \left(\frac{\pi}{\lambda}\right)^{1/2} - \alpha \right\}$$

$$E(\lambda) = \frac{\hbar^2 \lambda}{4m} - \alpha \sqrt{\frac{\lambda}{\pi}}$$

(4) $$\frac{dE}{d\lambda} = \frac{\hbar^2}{4m} - \frac{1}{2} \alpha \frac{1}{\sqrt{\pi \lambda}}$$

V-4

$dE/d\lambda = 0$ for $\lambda = \lambda_0$:

$$\frac{\hbar^2}{2m} = \alpha / \sqrt{\pi \lambda_0} \qquad \frac{2m}{\hbar^2} = \frac{\sqrt{\pi \lambda_0}}{\alpha}$$

$$\pi \lambda_0 = \left(\frac{2m\alpha}{\hbar^2}\right)^2 \qquad \lambda_0 = \frac{1}{\pi}\left(\frac{2m\alpha}{\hbar^2}\right)^2$$

$$E(\lambda_0) = \frac{\hbar^2}{4m} \frac{1}{\pi}\left(\frac{2m\alpha}{\hbar^2}\right)^2 - \alpha \frac{1}{\pi} \frac{2m\alpha}{\hbar^2}$$

$$= \frac{m\alpha^2}{\hbar^2}\left\{\frac{1}{\pi} - \frac{2}{\pi}\right\} = \frac{-m\alpha^2}{\hbar^2}\left(\frac{1}{\pi}\right)$$

$$= -\frac{m\alpha^2}{\hbar^2}(.3183)$$

Exact $-\frac{m\alpha^2}{\hbar^2}(.5000)$

Notice $E(\lambda_0) > E_{exact}$

This is no coincidence. Variational Energies are always bigger than the exact number.