S-2008

Problem 3: The Variational Principle: (10 Points)

If the case where you would like to calculate the ground state energy (E_g) for a system described by the Hamiltonian H but you are unable to solve the Schrodinger equation, the variational principle will give you an upper bound for the ground state energy.

For any normalized function Ψ, the variational principle states:

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

1.**(2 Points)** Prove the variational principle. i.e show that

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

Hint (Write $\Psi = \Sigma_n c_n \phi_n$ where ϕ_n are the (unknown) eigenfunctions of H)

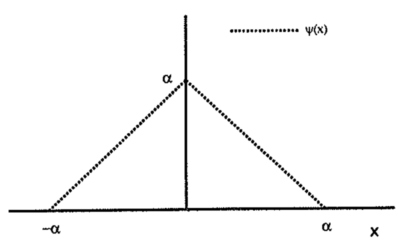
Now consider a specific case:
In the x-basis, a one-dimensional operator

$$\Omega = -\frac{d^2}{dx^2} + |x|$$

has an eigenvalue λ and an eigenfunction $\psi(x)$ with $\psi(x) \to 0$ for $|x| \to \infty$.
Let us choose an *unnormalized* trial function

$$\psi(x) = \langle x | \psi \rangle = \begin{cases} \alpha - |x|, & \text{for } |x| < \alpha, \text{ and} \\ 0, & \text{for } |x| > \alpha \end{cases}$$

where α is the variational parameter.



2. **(2 Points)** Find $\langle \psi | \psi \rangle$.

3. **(3 Points)** Find the expectation value of the operator Ω.

4. **(3 Points)** Determine the **best** bound on the lowest eigenvalue (λ) of the operator Ω with the trial function $\psi(x)$. (Note your answer cannot depend on α.)

S-2008

①

③

Ⓐ $\psi = \sum_n c_n \phi_n$

$\rightarrow \langle \psi | H | \psi \rangle =$

$\sum_n c_n^* \langle \phi_n | H \sum_m c_m | \phi_m \rangle$

$= \underbrace{\sum_n |c_n|^2}_{1} E_n$

$E_g \leq E_n$ by definition

$\rightarrow \sum_n |c_n|^2 E_n \geq E_g \underbrace{\sum_n |c_n|^2}_{1}$

$\rightarrow \boxed{\langle \psi | H | \psi \rangle \geq E_g}$

Ⓑ $\Omega \psi(x) = \lambda \psi(x)$

B Continued

$$\langle\psi|\psi\rangle = \int_{-\alpha}^{\alpha} (\alpha - |x|)\,dx$$

$$= 2\int_0^{\alpha} (\alpha - x)^2\,dx = 2\int_0^{\alpha} (\alpha^2 + x^2 - 2\alpha x)\,dx$$

$$= 2\left[\alpha^2 x\Big|_0^{\alpha} + \frac{x^3}{3}\Big|_0^{\alpha} - \alpha x^2\Big|_0^{\alpha}\right]$$

$$= 2\left[\alpha^3 + \frac{\alpha^3}{3} - \alpha^3\right]$$

$$= \boxed{\frac{2\alpha^3}{3} = \langle\psi|\psi\rangle}$$

C $$\langle\psi|\Omega|\psi\rangle = 2\int_0^{\alpha} (\alpha - x)\left[\frac{d^2}{dx^2} + x\right](\alpha - x)\,dx$$

$$= 2\int_0^{\alpha} (\alpha - x)\left[\cancel{-\frac{d^2}{dx}(\alpha - x)}^{\,0} + x(\alpha - x)\right]dx$$

$$= 2\int_0^{\alpha} (\alpha - x)\,x(\alpha - x)\,dx$$

$$= 2\int_0^{\alpha} \alpha^2 x + x^3 - 2\alpha x^2 = 2\left[\frac{\alpha^2 x^2}{2} + \frac{x^4}{4} - \frac{2\alpha x^3}{3}\right]_0^{\alpha}$$

(c) continued

$$= 2\left[\frac{\alpha^4}{2} + \frac{\alpha^4}{4} - \frac{2}{3}\alpha^4\right] = \alpha^4 + \frac{\alpha^4}{2} - \frac{4}{3}\alpha^4$$

$$= \frac{6+3-8}{6}\alpha^4$$

$$= \frac{1}{6}\alpha^4$$

$$\rightarrow \frac{\langle\psi|\Omega|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{3}{2\alpha^3}\,\frac{1}{6}\alpha^4 = \boxed{\frac{\alpha}{4}}$$

However, This is ~~wr~~ wrong

The reason is there is a discontinuity in the first derivative

For those $\displaystyle\int_{-\infty}^{\infty}\left|\frac{d^2\psi^2}{dx}\right| dx$

instead of $\displaystyle\int_{-\infty}^{\infty}\psi^*\frac{d^2}{dx^2}\psi\, dx$

$$\rightarrow \langle\psi|\Omega|\psi\rangle = -2\int_0^\alpha \frac{d^2}{dx^2}(\alpha-x)^2 dx$$

$$+2\int_0^\alpha x(\alpha-x)^2 dx$$

$$\rightarrow \alpha^2 + x^2 - 2\alpha x$$

$$\rightarrow -2x\Big|_0^\alpha + 2\left[\int_0^\alpha x\alpha^2 dx + \int_0^\alpha x^3 dx - \int_0^\alpha 2\alpha x\, dx\right]$$

C Continued

$$\rightarrow \underline{-2\alpha} + 2\left[\frac{x^2\alpha^2}{2}\Big|_0^\alpha + \frac{\alpha^4}{4}\Big|_0^\alpha - \frac{2\alpha x^2}{2}\Big|_0^\alpha \right]$$

$$2\frac{\alpha^4}{2} + \frac{2}{4}\alpha^4 - 2\alpha^4 = \frac{4+2-8}{4}\alpha^4$$

$$\underline{-\frac{\alpha^4}{2}}$$

$$\rightarrow \boxed{\frac{\langle\psi|\Omega|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{3}{2\alpha^3}\left(-2\alpha - \frac{\alpha^4}{2}\right) = -\frac{3}{\alpha^2} - \frac{3\alpha}{4}}$$

D

$$\rightarrow \frac{d\langle\psi|\Omega|\psi\rangle}{d\alpha} = \frac{6}{\alpha^3} - \frac{3}{4} = \emptyset$$

$$\rightarrow \frac{6}{\alpha^3} = \frac{3}{4} \rightarrow \frac{2}{\alpha^3} = \frac{1}{4}$$

$$\rightarrow \underline{8^{1/3} = \alpha}$$

$$\rightarrow \langle\psi|\Omega|\psi\rangle = \boxed{-\frac{3}{8^{2/3}} - \frac{3}{4}8^{1/3} \leq \lambda}$$

F-2011

PROBLEM 6: Variational Method

Consider a Hamiltonian H that may or may not be solved exactly. The variational theorem states that the expectation value of energy obtained from a trial wavefunction will always be greater than or equal to the ground state energy.

Consider a trial wave function ϕ consisting of two basis wavefunctions Ψ_1 and Ψ_2 such that

$$\phi = c_1\Psi_1 + c_2\Psi_2$$

where c_1 and c_2 are constants.

(a) Find the expectation value of the energy for this system. [1 point]

(b) Now assume $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle = 0$, $\langle\Psi_1|H|\Psi_2\rangle = \langle\Psi_2|H|\Psi_1\rangle$ and c_1 and c_2 are real. Determine a 2x2 matrix relationship for the best bound on the energy. [3 points]

(c) Now also assume Ψ_1 and Ψ_2 are orthonormal. Solve the matrix relationship you found in part (b) to determine 2 solutions for the best bound energy. [2 points]

(d) Note that there are 2 solutions to the best bound energy found in part (c). What additional constraint can you apply to remove one of the solutions? [2 points]

(e) Confirm your answer to part (c) by using a Simple Harmonic Oscillator Hamiltonian and setting Ψ_1 to be the ground state eigenfunction and Ψ_2 to be the first excited state eigenfunction of the Simple Harmonic Oscillator [2 points]

F-2011

6 A $\psi = c_1\psi_1 + c_2\psi_2$, if ψ_1 & ψ_2 are 2 basis wavefunctions

Assume $H\psi_1 = E_1\psi_1$

$H\psi_2 = E_2\psi_2$

$\rightarrow \langle\phi|H|\phi\rangle = \langle\phi|E|\phi\rangle$

$= \left[c_1^*\langle\psi_1| + c_2^*\langle\psi_2|\right] H \left[c_1|\psi_1\rangle + c_2|\psi_2\rangle\right]$

$$\boxed{\begin{aligned}\langle\phi|E|\phi\rangle &= c_1c_1^*\langle\psi_1|E_1|\psi_1\rangle + c_1^*c_2\langle\psi_1|E_2|\psi_2\rangle \\ &+ c_2^*c_1\langle\psi_2|E_1|\psi_1\rangle + c_2^*c_2\langle\psi_2|E_2|\psi_2\rangle\end{aligned}}$$

B
$$\boxed{\langle\phi|E|\phi\rangle = \begin{pmatrix} c_1^2\langle\psi_1|E_1|\psi_1\rangle & \emptyset \\ \emptyset & c_2^2\langle\psi_2|E_2|\psi_2\rangle \end{pmatrix} \geq E_{gs}}$$

C if orthonormal $\langle\psi_1|\psi_1\rangle = \emptyset$ & $c_1 = c_2 = \frac{1}{\sqrt{2}}$

$$\rightarrow \frac{1}{2}\begin{pmatrix} E_1 - E & \emptyset \\ \emptyset & E_2 - E \end{pmatrix}$$

$\rightarrow (E_1 - E)(E_2 - E) = \emptyset$

$E_1E_2 - E_1E - EE_2 + E^2 = \emptyset$

$E^2 + E(-E_1 - E_2) + E_1E_2$

C Continued

$$E = \frac{E_1 + E_2 \pm \sqrt{(-E_1 - E_2)^2 - 4E_1E_2}}{2}$$

$(-E_1 - E_2)(-E_1 - E_2)$

$E_1^2 +$

$$= \frac{E_1 + E_2 \pm \sqrt{E_1^2 + E_2^2 + 2E_1E_2 - 4E_1E_2}}{2}$$

$\sqrt{(E_1 - E_2)^2}$

$$= \frac{E_1 + E_2 \pm (E_1 - E_2)}{2} = \frac{2E_1}{2} = \boxed{E_1 \text{ or } E_2}$$

D ?

E Should be easy?

F-2009

Problem 2: Variational Method (10 points) 2

Let us consider the hydrogen atom without spin. The Hamiltonian is

$$H = \frac{P^2}{2m} - \frac{C}{r} \, . \tag{1}$$

Since the ground state is an S state the wave function must be spherically symmetrical. Suppose you could not solve this problem exactly. Estimate the ground state wave function with a Gaussian:

$$\psi(\vec{r}) = N e^{-r^2/b^2} \, .$$

a) Compute the normalization constant N so that $\psi(\vec{r})$ is correctly normalized. (2 pts)

b) Evaluate the expectation value of H in this state. (3 pts)

c) Find the best estimate for E_0 by applying the variational method. (4 pts)

d) The true ground state energy is

$$E_0 = -\frac{1}{2}(C^2 m) \, .$$

How much does your estimate in (c) differ from the correct answer? (1 pt)

F-2009

(2) $H = \frac{p^2}{2m} - \frac{c}{r}$

$\psi(\vec{r}) = Ne^{-r^2/b^2}$

(A) $1 = \int_{\text{All Space}} \psi^2 d^3x = N^2 \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-2r^2/b^2} r^2 \sin\theta \, dr\, d\theta\, d\phi$

$$= 4\pi N^2 \underbrace{\int_0^\infty e^{-2r^2/b^2} r^2 dr}_{\frac{\Gamma[(2+1)/2]}{2\left(\frac{2}{b^2}\right)^{3/2}}}$$

$\Gamma(1+\frac{1}{2}$

$$\frac{\Gamma[(2+1)/2]}{2\left(\frac{2}{b^2}\right)^{3/2}} = \frac{\frac{1}{2}\sqrt{\pi}}{\frac{2^{5/2}}{b^3}}$$

$\frac{2}{2} + \frac{7}{2}$

$\frac{5}{2}$

$$= \frac{b^3\sqrt{\pi}}{2^{7/2}}$$

$$= \frac{2^2 b^3 \pi \pi^{1/2}}{2^{7/2}} = \frac{b^3 \pi^{3/2}}{2^{3/2}} N^2 = 1$$

$$\rightarrow \boxed{N = \frac{2^{3/4}}{b^{3/2}\pi^{3/4}}}$$

$\cancel{\frac{4}{2} - \frac{7}{2}} = \cancel{\frac{3}{2}} - \frac{3}{2}$

$\frac{2}{2} + \frac{1}{2} = \frac{3}{2}$

B $\langle H \rangle = \langle T \rangle + \langle V \rangle$

$\rightarrow \frac{p^2}{2m} = \frac{-\hbar^2}{2m} \nabla^2$

$= \frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(\underbrace{r^2\frac{\partial \psi}{\partial r}}\right)\right]$

$r^2\left[N\left(-\frac{2r}{b^2}\right)e^{-r^2/b^2}\right]$

$\frac{\partial}{\partial r}\left[-\frac{2N}{b^2} r^3 e^{-r^2/b^2}\right]$

$= -\frac{2N}{b^2}\left[3r^2 e^{-r^2/b^2} - \frac{2r^4}{b^2} e^{-r^2/b^2}\right]$

$\rightarrow \times \frac{1}{r^2} = \frac{-2N}{b^2}\left[3e^{-r^2/b^2} - \frac{2r^2}{b^2} e^{-r^2/b^2}\right]$

$\rightarrow \frac{p^2}{2m}\psi = \frac{\hbar^2 N}{mb^2}\left[3e^{-r^2/b^2} - \frac{2r^2}{b^2} e^{-r^2/b^2}\right]$

$\rightarrow \langle T \rangle = \frac{\hbar^2 N^2 4\pi}{mb^2}\left[3\int_0^\infty e^{-2r^2/b^2} r^2 dr - \frac{2}{b^2}\int_0^\infty r^4 e^{-2r^2/b^2} dr\right]$

$\frac{\Gamma((2+1)/2]}{2a^{(3/2)}}$ $\qquad$ $\frac{\Gamma[(4+1)/2]}{2a^{(5/2)}}$

$\frac{\frac{\sqrt{\pi}}{2}}{2\left(\frac{2}{b^2}\right)^{3/2}}$ $\qquad$ $\frac{\frac{3\sqrt{\pi}}{8}}{2\left(\frac{2}{b^2}\right)^{5/2}}$ $\quad 2+\frac{1}{2}$

B Continued

$$\langle T\rangle = \frac{\hbar^2 N^2 4\pi}{mb^2}\left[\frac{3\sqrt{\pi}\,b^3}{4(2^{3/2})} - \frac{2}{b^2}\frac{3\sqrt{\pi}\,b^5}{16(2^{5/2})}\right]$$

$$= \frac{\hbar^2 \cancel{4\pi}}{mb^2}\frac{3}{\cancel{4}}\frac{\cancel{\sqrt{\pi}}\,\cancel{b^3}}{\cancel{2^{3/2}}}\frac{\cancel{2^{3/2}}}{\cancel{b^3}\cancel{4}\cancel{\pi^{3/2}}} \quad \left(\frac{3\hbar^2}{mb^2}\right)$$

$$- \frac{\hbar^2 4\cancel{\pi}}{mb^2}\frac{\cancel{2}}{\cancel{b^2}}\frac{3\cancel{\sqrt{\pi}}\,\cancel{b^5}}{16(\cancel{2^{5/2}})}\frac{\cancel{2^{3/2}}}{\cancel{b^3}\cancel{\pi^{3/2}}} \quad \left(\frac{3\hbar^2}{16mb^2}\right)$$

$$= \left[\frac{(16)(3)}{16} - \frac{3}{16}\right]\frac{\hbar^2}{mb^2}$$

$16 \times 3 = 48$

$48 - 3 = 45$

$$\frac{45}{16}\frac{\hbar^2}{mb^2}$$

$$\langle V\rangle = N^2 4\pi c^2 \underbrace{\int_0^\infty e^{-2r^2/b^2}}_{\frac{1}{2}\sqrt{\frac{\pi}{(2/b^2)}} = \frac{b}{2}\sqrt{\frac{\pi}{2}} = \frac{b\,\pi^{1/2}}{2^{3/2}}}$$

$\boxed{\text{STUPID MISTAKE}}$

$\boxed{\text{Its } -\frac{c}{r} \text{ NOT } \frac{c^2}{r^2}}$

$$= \frac{4\cancel{\pi^{3/2}}c^2}{\cancel{2^{3/2}}}\frac{\cancel{2^{3/2}}\,b}{b^{2}\cancel{b}\cancel{\pi^{3/2}}} = \frac{4c^2}{b^2}$$

$$\rightarrow \langle H\rangle = \frac{45}{16}\frac{\hbar^2}{mb^2} + \frac{4c^2}{b^2}$$

C $\frac{d\langle H\rangle}{db} = \emptyset \rightarrow -\frac{45}{8}\frac{\hbar^2}{mb^3} - \frac{8c^2}{b^3} = \emptyset$

easy once you do this

F-2010

PROBLEM 5: Variational Method

In the x-basis, the Hamiltonian for a hydrogen atom is

$$\begin{aligned} H &= \frac{P^2}{2m} - \frac{e^2}{r} \\ &= -\frac{\hbar^2}{2m}\nabla^2 - \frac{e}{r}. \end{aligned}$$

Let us choose

$$\psi_\alpha(r) = e^{-\alpha r^2}, \quad \alpha > 0$$

as a trial wave function for the ground state.

(a) [2 points] Find $\langle \psi_\alpha | \psi_\alpha \rangle$. (**N.B.** This wave function is not normalized.)

(b) [4 points] Find the expectation value of the Hamiltonian $\langle H \rangle$.

(c) [4 points] Determine the best bound on the energy for the ground state of this system using the variational method and the trial wave function given above.

F-2010

5

$\varphi_\alpha = e^{-\alpha r^2}$

A $\langle \varphi_\alpha | \varphi_\alpha \rangle = \int_0^\infty e^{-2\alpha r^2} r^2 \sin\theta \, dr \, d\theta \, d\phi$

$$= 4\pi \underbrace{\int_0^\infty e^{-2\alpha r^2} r^2 \, dr}_{\frac{\Gamma(1+\frac{1}{2}) = \frac{1}{2}\sqrt{\pi}}{2(2\alpha)^{3/2}}}$$

$$= \frac{\pi \, \pi^{1/2}}{(2\alpha)^{3/2}} = \boxed{\left(\sqrt{\frac{\pi}{2\alpha}}\right)^3}$$

$\frac{2}{2} - \frac{3}{2} = -\frac{1}{2}$

B Normalize $\varphi_\alpha \rightarrow \langle \varphi_\alpha | \varphi_\alpha \rangle = 1$

$\rightarrow \left(\frac{\pi}{2\alpha}\right)^{3/2} A^2 = 1$

$\rightarrow A^2 = \left(\frac{2\alpha}{\pi}\right)^{3/2} = \left(\frac{2\alpha}{\pi}\right)^{3/4} = A$

$\rightarrow \varphi_\alpha = \left(\frac{2\alpha}{\pi}\right)^{3/4} e^{-\alpha r^2}$

$\to \frac{6}{4} = \frac{3}{2}$

B Continued

$$\to -\frac{\hbar^2}{2m}\nabla^2\psi = -\frac{\hbar^2}{2m}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right)$$

$$\to \frac{\partial \psi}{\partial r} = A(-2r\alpha)e^{-\alpha r^2}$$

$$\to \frac{\partial}{\partial r}\left(-2A\alpha r^3 e^{-\alpha r^2}\right)$$

$$= -6A\alpha r^2 e^{-\alpha r^2} + 4A\alpha r^4 e^{-\alpha r^2}$$

$$\to \nabla^2 = -\frac{\hbar^2 A}{m} e^{-\alpha r^2}\left[2\alpha r^2 - 3\alpha\right]$$

$$\to \langle T\rangle = -\frac{\hbar^2 A^2 \alpha}{m}(4\pi)\int_0^\infty e^{-2\alpha r^2}(2r^2-3)r^2\,dr$$

This is key $\to$ $\boxed{\text{Take } \nabla^2 \text{ outside integral}}$

The rest of this problem is straight forward

F-2014

PROBLEM 6: Variational approach

A particle with mass, m, moving in one dimension finds itself in a potential given by,

$$V = \infty \quad \text{for} \quad x < 0$$

and

$$V = \beta x^3 \quad \text{for} \quad x > 0$$

where β is a positive constant.

a) Find an approximation to the ground state energy, using the trial wavefunction

$$\Psi = 0 \quad \text{for} \quad x < 0$$

and

$$\Psi = Cxe^{-\alpha x} \quad \text{for} \quad x > 0.$$

where C and α are positive constants. (5 Points)

b) Would you expect the exact ground state energy to be less than your answer to part (a), or greater than it? Justify. (3 Points)

c) How would you go about finding an excited state in this system using the same approach? (2 Points)

Hint: $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, for $a > 0$.

①

F-2014

⑥ $V = \infty$ For $x < \emptyset$

$= \beta x^3 \quad x > \emptyset$

Ⓐ $\psi = 0 \quad x < \emptyset$

$= C x e^{-\alpha x} \quad x > \emptyset$

$$\langle \psi | H | \psi \rangle = \langle \psi | \frac{p^2}{2m} | \psi \rangle + \langle \psi | \beta x^3 | \psi \rangle$$

$$\rightarrow \quad p = -i\hbar \frac{\partial}{\partial x} \quad \rightarrow \quad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

$$\rightarrow \langle \psi | \frac{p^2}{2m} | \psi \rangle = \frac{-\hbar^2}{2m} \int_0^\infty C x e^{-\alpha x} \frac{\partial^2}{\partial x^2} C x e^{-\alpha x} \, dx$$

$$= -\frac{C^2 \hbar^2}{2m} \int_0^\infty -2\alpha x e^{-2\alpha x} + \alpha^2 x^2 e^{-2\alpha x} \, dx$$

$$\rightarrow \frac{\partial^2}{\partial x^2}\left(x e^{-\alpha x}\right) = \frac{\partial}{\partial x}\left[e^{-\alpha x} - \alpha x e^{-\alpha x}\right]$$

$$= -\alpha e^{-\alpha x} - \alpha e^{-\alpha x} + \alpha^2 x e^{-\alpha x}$$

$$= -2\alpha e^{-\alpha x} + \alpha^2 x e^{-\alpha x}$$

A Continued

$$\rightarrow \frac{\alpha c^2 \hbar^2}{m}\int_0^\infty x e^{-2\alpha x}\,dx = \frac{\alpha c^2 \hbar^2}{m}\left[\frac{\Gamma(2)}{(2\alpha)^2}\right]$$

$$= \frac{c^2\hbar^2}{4\alpha m}$$

$$\rightarrow -\frac{\alpha^2 c^2 \hbar^2}{2m}\int_0^\infty x^2 e^{-2\alpha x}\,dx = -\frac{\alpha^2 c^2 \hbar^2}{2m}\left[\frac{\Gamma(2+1)}{(2\alpha)^3}\right]$$

$$= -\frac{\alpha^2 c^2 \hbar^2}{8m\alpha^3}$$

$$= -\frac{c^2\hbar^2}{8m\alpha}$$

$$\rightarrow \langle\psi|T|\psi\rangle = \frac{1}{8}\frac{c^2\hbar^2}{\alpha m}$$

$2\cdot 2 = 4\cdot 2 = 8\cdot 2$

$= 16\times 2 =$

$\frac{2}{32}$

$\times\frac{2}{64}$

$$\rightarrow \langle\psi|V|\psi\rangle = \int_0^\infty c^2 x^2 e^{-2\alpha x}\beta x^3\,dx$$

$$= c^2\beta\int_0^\infty x^5 e^{-2\alpha x}\,dx = \frac{\Gamma(5+1)}{(2\alpha)^6}$$

$120 \div 60 \div 2 = 30 \div 15$

$\div 2$

$32 \div 16 \quad 8$

$$= 5\cdot 4\cdot 3\cdot 2\cdot 1$$

$= 20$

$\frac{3}{60}$

$\frac{2}{120}$

$$= \frac{c^2\beta(120)}{64\,\alpha^6} = \frac{15}{8}\frac{c^2\beta}{\alpha^6}$$

A Continued

$$\langle \psi | \psi \rangle = 1 = \int_0^\infty C^2 x^2 e^{\cancel{\alpha x} -2\alpha x} dx$$

$$= \frac{\Gamma(2+1)}{(2\alpha)^3} = \frac{2C^2}{8\alpha^3} = 1$$

$$\rightarrow C = \sqrt{4\alpha^3} = 2\alpha^{3/2}$$

$$\rightarrow E_{gs} \leq \frac{1}{8}\frac{4\alpha^3\hbar^2}{\alpha m} + \frac{15}{8}\frac{(4)\alpha^3\beta}{\alpha^6}$$

$$\leq \frac{1}{2}\frac{\alpha^2\hbar^2}{m} + \frac{15}{2}\frac{\beta}{\alpha^3}$$

→ Minimized with respect to constants in trial function to get tightest bound

$$\frac{15}{3} \quad \frac{}{45}$$

$$\frac{\partial E_{gs}}{\partial \alpha} = \frac{\alpha\hbar^2}{m} - 15\frac{3}{2}\frac{\beta}{\alpha^4} = \emptyset$$

$$= \frac{\alpha\hbar^2}{m} - \frac{45}{2}\frac{\beta}{\alpha^4} = \emptyset \rightarrow \alpha^5\frac{\hbar^2}{m} = \frac{45}{2}\beta$$

$$\rightarrow \alpha = \left(\frac{m}{\hbar^2}\frac{45}{2}\beta\right)^{1/5}$$

$$\rightarrow \boxed{E_{gs} \leq \frac{1}{2}\left(\frac{m}{\hbar^2}\frac{45}{2}\beta\right)^{2/5}\frac{\hbar^2}{m} + \frac{15}{2}\beta\left(\frac{m}{\hbar^2}\frac{45}{2}\beta\right)^{-3/5}}$$

B $\langle\psi|H|\psi\rangle = \sum_{m,n} C_m \psi_m^* H C_n \psi_n$

$$= \sum_{m,n} C_m C_n \psi_m^* E_n \psi_n = \sum_{m,n} C_m C_n E_n \underbrace{\psi_m^* \psi_n}_{\delta_{m,n}}$$

$$= \sum_n |C_n|^2 E_n$$

$$\rightarrow \langle\psi|\psi\rangle = \sum_{mn} C_m C_n \underbrace{\psi_m^* \psi_n}_{\delta_{mn}} = 1 \rightarrow \sum_n |C_n|^2 = 1$$

E_{gs} is the smallest eigenvalue

$$E_{gs} \leq E_n$$

$$\langle\psi|H|\psi\rangle = \underbrace{\sum_n |C_n|^2}_{1} E_n \quad = \boxed{\begin{array}{c} E_n \geq E_{gs} \\ \shortparallel \\ \langle\psi|H|\psi\rangle \end{array}}$$

C Find a new trial wave function ψ_1 such that

$\langle\psi_1|\psi_0\rangle = \phi$ Then follow same procedure as A