THE VARIATIONAL METHOD

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④ Minimize over a_i $\longrightarrow$ E_ψ^{min}

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③ Calculate $E_\psi(a_i) = \langle\Psi(a_i)|H|\Psi(a_i)\rangle$

④ Minimize over $a_i \longrightarrow E_\psi^{min}$

Result: $E_0 \leq E_\psi^{min}$ ← this is our estimate

The Variational Method

Question: In a spin $\frac{1}{2}$ system with Hamiltonian H Katie evaluates $\langle x|H|x\rangle$ for $|x\rangle = |\uparrow\rangle + |\downarrow\rangle$ and finds $0.2\,eV$. She can conclude that:

1. $E_0 \leq 0.2\,eV$
2. $E_0 \geq 0.2\,eV$
3. $E_0 \leq 0.1\,eV$
4. $E_0 \geq 0.1\,eV$
5. $E_0 \leq 0.4\,eV$
6. $E_0 \geq 0.4\,eV$

The Variational Method

Question: For a quantum system with 3-dimensional Hilbert space and Hamiltonian represented as

$$H = E\begin{pmatrix} 4 & 2 & 7 \\ 2 & 1 & 3 \\ 7 & 3 & 5 \end{pmatrix}$$

what is the upper bound that we can place on the ground state energy by considering a trial state $|\Psi\rangle$ represented as $\begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix}$ for some fixed θ?

EXTRA: What is the best we can do if we consider all possible θ?

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what is the upper bound that we can place on the ground state energy by considering a trial state $|\Psi\rangle$ represented as $\begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix}$ (for some fixed θ).

① $4E\cos^2\theta$

② $4E\cos^2\theta + E\sin^2\theta$

③ $E\sin^2\theta$

④ $4E\cos^2\theta + 4E\cos\theta\sin\theta + E\sin^2\theta$

⑤ E

THE VARIATIONAL METHOD

Question: A particle in 1D has a Hamiltonian

$$H = \frac{p^2}{2m} + \lambda x^4$$

If we use a properly normalized trial wavefunction $\psi(x)$ for our variational method, what is the bound on E_0?

THE VARIATIONAL METHOD

Question: A particle in 1D has a Hamiltonian

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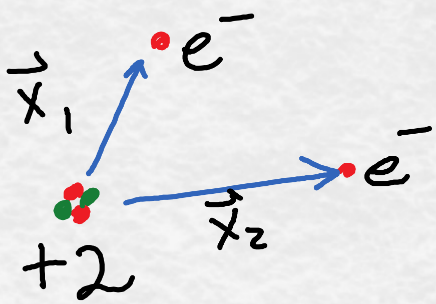
If we use a properly normalized trial wavefunction $\psi(x)$ for our variational method, what is the bound on E_0?

1. $\int dx \, \lambda x^4 |\psi(x)|^2$
2. $\int dx \left\{ -\frac{\hbar^2}{2m} \psi^*(x) \psi''(x) + \lambda x^4 |\psi(x)|^2 \right\}$
3. $\int dx \, \lambda |\psi(x)|^4$
4. $\frac{1}{2}\hbar\omega$

THE VARIATIONAL METHOD: Helium atom



Discussion questions (breakout groups)

① What is the "position space" description of the two electrons in a Helium atom?

e.g.: two wavefunctions $\psi_1(\vec{x}), \psi_2(\vec{x})$

one wavefunction $\psi(\vec{x}_1, \vec{x}_2)$

wavefunctions $\psi_1(\vec{x}_1, \vec{x}_2), \psi_2(\vec{x}_1, \vec{x}_2)$

② What is the Hamiltonian that describes the two electrons in a Helium atom?

(hint: it's also the energy operator)

THE VARIATIONAL METHOD

Helium atom Hamiltonian:

$$H = \frac{p_1^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1|} + \frac{p_2^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_2|} + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$$

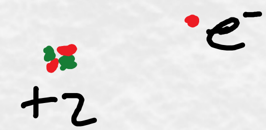
The Variational Method

Helium atom Hamiltonian:

$$H = \frac{p_1^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1|} \quad \Bigg\} \text{ Hamiltonian for } He^+ \text{ ion}$$

$$+ \frac{p_2^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_2|}$$

$$+ \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$$



Ground state is $\psi^{Z}_{100}(\vec{x})$

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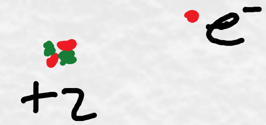
Helium atom Hamiltonian:

$$H = \underbrace{\frac{p_1^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1|}}_{\text{Hamiltonian for } He^+ \text{ ion}}$$

$$+ \frac{p_2^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_2|}$$

$$+ \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$$



Ground state is

$$\psi_{100}^{Z=2}(\vec{x}) = e^{-Zr/a} \times N$$

Simple trial state: both electrons independently in this state.

Q: Does that mean:

① $\psi(\vec{x}_1, \vec{x}_2) = \psi_{100}^{Z=2}(\vec{x}_1)\,\psi_{100}^{Z=2}(\vec{x}_2)$

② $\psi(\vec{x}_1, \vec{x}_2) = \psi_{100}^{Z=2}(\vec{x}_1) + \psi_{100}^{Z=2}(\vec{x}_2)$

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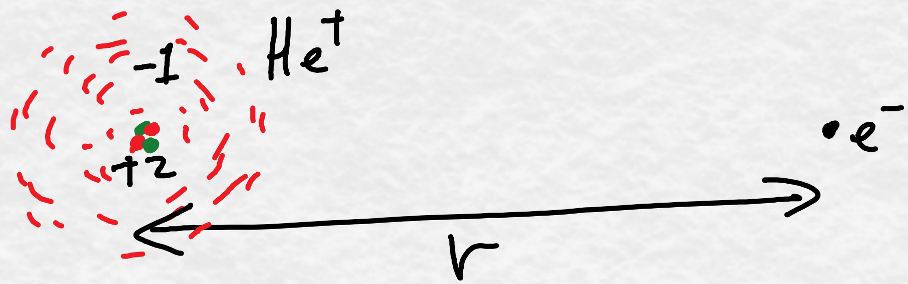
TRIAL STATE #2: $\psi(\vec{x}_1, \vec{x}_2) = \psi^{Z}_{100}(\vec{x}_1)\,\psi^{Z}_{100}(\vec{x}_2)$

arbitrary parameter.

Motivation:



If the first electron is in a spherically symmetric configuration about the He nucleus, what potential is felt by the second electron when it is far away?

1. $-\dfrac{1}{4\pi\varepsilon_0}\dfrac{e^2}{r}$

2. $-\dfrac{1}{4\pi\varepsilon_0}\dfrac{2e^2}{r}$

3. $\dfrac{1}{4\pi\varepsilon_0}\dfrac{e^2}{r}$

4. $\dfrac{1}{4\pi\varepsilon_0}\dfrac{2e^2}{r}$

5. 0

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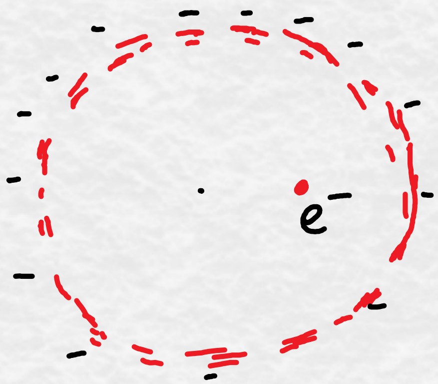
Q: The electron shown is inside a spherically symmetric shell of negative charge.



The force felt by the electron is

① To the left

② To the right

③ Zero.

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Helium atom Hamiltonian:

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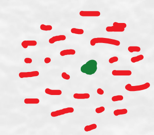
$$+ \frac{p_2^2}{2m} - \frac{2e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_2|}$$

$$+ \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$$



Summary: each electron partly "screens" charge of nucleus; this motivates trial wavefn.

$$\psi_{100}^{Z}(\vec{x}_1)\,\psi_{100}^{Z}(\vec{x}_2) \qquad 1 \leq Z \leq 2$$