REMEMBER: FOR APPLICATION OF PERTURBATION THEORY, PERTURBED AND UNPERTURBED EIGENVALUES AND EIGENSTATES ARE NOT TOO DIFFERENT

VARIATIONAL METHOD OR RAYLEIGH - RITZ METHOD

APPROXIMATE METHOD FOR FINDING [UPPER BOUND] VALUES FOR EIGENENERGIES [USUALLY THE GROUND STATE] IF HAMILTONIAN IS KNOWN, BUT EIGENVALUES AND EIGENSTATES CAN NEITHER BE CALCULATED EXACTLY, NOR APPROXIMATELY [E.G., IF PERTURBATION THEORY IS NOT SUFFICIENTLY ACCURATE]

MEANING:

$$\underbrace{H}_{\text{KNOWN}} \; \underbrace{|\psi_n\rangle}_{\text{UNKNOWN}} = \overbrace{E_n}^{\text{UNKNOWN}} |\psi_n\rangle \qquad \text{CANNOT BE SOLVED}$$

WE KNOW THAT THE SET OF ψ_n IS ORTHONORMAL; THIS IS A GENERAL PROPERTY, INDEPENDENT OF EXPLICIT KNOWLEDGE OF $|\psi_n\rangle$

VARIATIONAL METHOD WAS BASIS FOR 2 NOBEL PRIZES:

- BARDEEN, COOPER, SCHRIEFFER: (BCS) THEORY OF SUPERCONDUCTIVITY [NOBEL PRIZE 1972]
- LAUGHLIN, STÖRMER, TSUI: THEORY OF FRACTIONAL QUANTUM HALL EFFECT [NOBEL PRIZE 1998]

INSTEAD OF SCHRÖDINGER EQUATION, CONSIDER FOR AN ARBITRARY WAVE FUNCTION, ϕ, THE ENERGY EXPECTATION VALUE :

$$E[\phi] = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

"FUNCTIONAL"; E DEPENDS EXPLICITLY ON ϕ AND IMPLICITLY ON OTHER PARAMETERS ENTERING IN ϕ

(i) SUPPOSE YOU KNOW $|\psi_n\rangle$ ALREADY AND YOU PICK $|\phi\rangle = |\psi_n\rangle$

$$\Rightarrow \quad E[\phi] = \frac{\langle \psi_n | H | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} = E_n$$ EXACT EIGENVALUE

(ii) SUPPOSE WE DO NOT KNOW $|\psi_n\rangle$; IF WE PICK AN ARBITRARY TRIAL FUNCTION, $|\phi\rangle$, DESCRIBING THE SYSTEM, WE CAN EXPRESS IT AS A SUPERPOSITION OF THE ORTHONORMAL SET $|\psi_n\rangle$: $\quad |\phi\rangle = \sum_n c_n |\psi_n\rangle$

$$\Rightarrow \quad E[\phi] = \frac{\langle \sum_m c_m \psi_m | H | \sum_n c_n \psi_n \rangle}{\langle \sum_m c_m \psi_m | \sum_n c_n \psi_n \rangle} = \frac{\langle \sum_m c_m \psi_m | E_n | \sum_n c_n \psi_n \rangle}{\langle \sum_m c_m \psi_m | \sum_n c_n \psi_n \rangle}$$

$$= \frac{\sum_m \sum_n c_m^* E_n c_n \langle \psi_m | \psi_n \rangle}{\sum_m \sum_n c_m^* c_n \langle \psi_m | \psi_n \rangle} = \frac{\sum_n E_n |c_n|^2}{\sum_n |c_n|^2} \geq \frac{E_0 \sum_n |c_n|^2}{\sum_n |c_n|^2} = E_0$$

SINCE $E_0 \leq E_n$

[DEFINITION OF GROUND STATE]

$$E_0 |c_0|^2 + E_1 |c_1|^2 + \dots$$
$$\vee$$
$$E_0 |c_0|^2 + E_0 |c_1|^2 + \dots$$

$\Rightarrow$ FUNCTIONAL $E[\phi]$ GIVES AN UPPER LIMIT APPROXIMATION FOR THE GROUND STATE ENERGY

RAYLEIGH - RITZ METHOD FOR APPROXIMATE CALCULATION OF E_0:

(1) USE TRIAL FUNCTION $|\phi\rangle$ THAT DEPENDS ON ADJUSTABLE PARAMETERS α_i

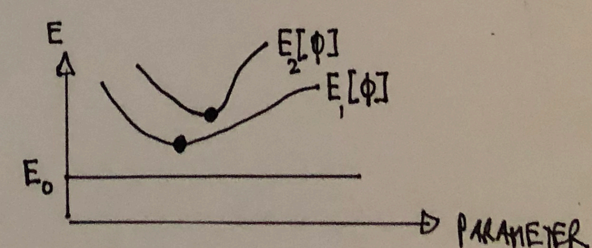
(2) CALCULATE $E[\phi]$, WHICH WILL DEPEND ON ADJUSTABLE PARAMETERS α_i

(3) MINIMIZE $E[\phi]$ WITH RESPECT TO THESE PARAMETERS,

$$\frac{\partial E[\phi]}{\partial \alpha_1} = \frac{\partial E[\phi]}{\partial \alpha_2} = \ldots = 0$$

TO FIND BEST APPROXIMATION OF E_0 AND ψ_n ALLOWED BY THE FORM OF TRIAL FUNCTION ϕ

GROUND STATE ENERGY AND EIGENSTATE ARE ESTIMATED WITHOUT EXPLICITLY SOLVING SCHRÖDINGER EQUATION



HOW TO PICK TRIAL FUNCTIONS:

- LET YOUR PHYSICS INTUITION GUIDE YOU
- SHOULD CONTAIN AS MANY FEATURES OF EXACT WAVEFUNCTION AS POSSIBLE [E.G., USE SYMMETRY ARGUMENTS, NUMBER OF NODES, SMOOTHNESS, ...]
- SHOULD RESULT IN REASONABLY SIMPLE CALCULATIONS
- IF HIGH PRECISION IS REQUIRED, SHOULD CONTAIN SEVERAL [MANY] ADJUSTABLE PARAMETERS; THE MORE PARAMETERS, THE LARGER CHANCE THAT A SMALLER VALUE OF $E[\phi]$ CAN BE FOUND [LOWER UPPER LIMIT]

CAREFUL:

THERE IS NO WAY TO JUDGE HOW CLOSE YOUR RESULT IS TO THE ACTUAL VALUE!

YOU CAN TRY TO USE SEVERAL DIFFERENT TRIAL FUNCTIONS, MINIMIZE EACH, AND SEE WHICH ONE GIVES THE LOWEST E_0

HELPFUL HINT # 1:

SUMMARY OF CENTRAL POTENTIAL EXPRESSIONS:

HW #3 LAPLACIAN

ROTATIONAL KINETIC E

$$\boxed{\frac{p^2}{2m} = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right] + \frac{\vec{L}^2}{2mr^2}}$$

RADIAL KINETIC E

$$\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

HAMILTONIAN CAN ALSO BE WRITTEN AS:

$$H = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}r\right] - \frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V$$

FORM I USE IN EXAMPLES / HW SOLUTIONS

TWO FORMS ARE EQUIVALENT:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) = \frac{1}{r^2}\left[2r\frac{\partial}{\partial r} + r^2\frac{\partial^2}{\partial r^2}\right] = \frac{2}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} = \frac{1}{r}\left[\frac{\partial}{\partial r} + \frac{\partial}{\partial r} + r\frac{\partial^2}{\partial r^2}\right]$$

$$= \frac{1}{r}\frac{\partial}{\partial r}\Big[\underbrace{1 + r\frac{\partial}{\partial r}}_{\frac{\partial}{\partial r}r}\Big]$$

[GIVE OPERATOR EXPRESSIONS A TEST FUNCTION, $f(r)$, THAT CAN BE REMOVED AFTER CALCULATION]

NORMALIZATION :

$$\langle \psi | \psi \rangle = \langle RY | RY \rangle = \int dV \, |RY|^2$$

$\psi = R(r)\, Y(\theta, \phi)$

$$dV = r^2 dr \underbrace{\sin\theta \, d\theta \, d\phi}_{d\Omega}$$

$$\langle \psi | \psi \rangle = \int_0^\infty r^2 dr \, |R(r)|^2 \underbrace{\int_{4\pi} d\Omega \, |Y(\theta, \phi)|^2}_{=1}$$

HELPFUL HINT #2

IF TRIAL FUNCTION HAS A KINK [FIRST DERIVATIVE DISCONTINUOUS AT CERTAIN LOCATION], BE VERY CAREFUL WITH EXPECTATION VALUE OF KINETIC ENERGY;

CARELESS APPLICATION OF

$$-\langle \psi | \frac{\hbar^2}{2m} \frac{d^2}{dx^2} | \psi \rangle = \boxed{-\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \psi^*(x) \frac{d^2}{dx^2} \psi(x)\, dx}$$

2ND ORDER DERIVATIVE

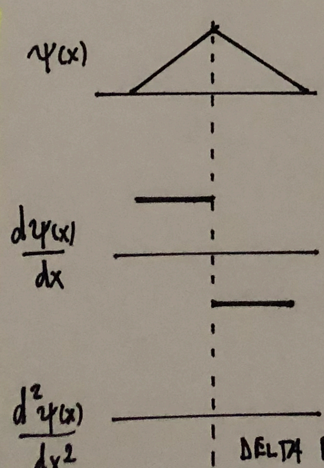
MAY WRONGLY YIELD ZERO OR NEGATIVE KINETIC ENERGIES; SAFER TO USE:

SQUARE OF 1ST ORDER DERIVATIVE

$$-\langle \psi | \frac{\hbar^2}{2m} \frac{d^2}{dx^2} | \psi \rangle = \underbrace{\boxed{\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \left| \frac{d\psi(x)}{dx} \right|^2 dx}}_{\text{ALWAYS POSITIVE}}.$$

[$\frac{d}{dx}$ IS NOT HERMITIAN]

[TRUE WAVEFUNCTION CANNOT HAVE KINKS:
→ $T = -\hbar^2/2m\, \nabla^2$ WOULD BECOME INFINITE]



DELTA FUNCTION [INFINITE SLOPE OF $d\psi(x)/dx$]

EQUIVALENCE OF EXPRESSIONS [INTEGRATION BY PARTS]:

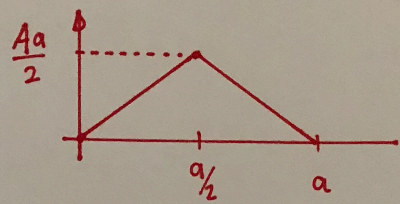
$$\int_{-\infty}^{+\infty} \left| \overset{v'\,u}{\frac{d\psi(x)}{dx}} \right|^2 dx$$

$$= \underbrace{\left[\overset{v}{\psi^*(x)} \overset{u}{\frac{d\psi(x)}{dx}} \right]_{-\infty}^{+\infty}}_{\emptyset \text{ AS } x \to \pm\infty \text{ FOR BOUND STATES}} - \int_{-\infty}^{+\infty} \overset{v}{\psi^*(x)} \overset{u'}{\frac{d^2}{dx^2} \psi(x)}\, dx$$

$$= -\int_{-\infty}^{+\infty} \psi^*(x) \frac{d^2}{dx^2} \psi(x)\, dx$$

$\boxed{\text{EXAMPLE}}$ [EXAMPLE 7.3 GRIFFITHS; BUT WE WILL SOLVE IT DIFFERENTLY]

FIND UPPER BOUND ON GROUND STATE ENERGY OF 1D INFINITE SQUARE WELL USING A TRIANGULAR WAVE FUNCTION:



$$\phi(x) = \begin{cases} Ax & , \ 0 \le x \le a/2 \\ A(a-x) & , \ a/2 \le x \le a \\ 0 & , \ \text{OTHERWISE} \end{cases}$$

FOR ACTUAL WAVEFUNCTION, OF COURSE, $\frac{d}{dx^2}\psi$ MUST BE SINGLE-VALUED AND FINITE

WHAT DO WE REASONABLY KNOW ABOUT THE PROBLEM:

- LOWEST ENERGY ψ SHOULD HAVE NO NODE
- ψ DISAPPEARS AT BOUNDARIES
- ψ IS SYMMETRIC [POTENTIAL SYMMETRIC]

TASKS: (1) FIND NORMALIZATION CONSTANT $\langle \phi | \phi \rangle$

(2) FIND $E[\phi] = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$

[PROVIDE INTEGRAL →]

HELP: $$\int_{a/2}^{a} (a-x)^2 dx = \left[\frac{1}{3} x (3a^2 - 3ax + x^2) \right]_{a/2}^{a}$$

[NOT NECESSARILY REQUIRED]

$$1 = \langle \phi | \phi \rangle = \int \phi^* \phi \, dx = \int_0^{a/2} (Ax)^2 dx + \int_{a/2}^{a} [A(a-x)]^2 dx$$

$$= A^2 \Bigg[\underbrace{\int_0^{a/2} x^2 dx}_{\left[\frac{1}{3}x^3\right]_0^{a/2}} + \boxed{\underbrace{\int_{a/2}^{a} (a-x)^2 dx}_{\left[\frac{1}{3}x(3a^2-3ax+x^2)\right]_{a/2}^{a}}} \Bigg]$$

PROVIDE INTEGRAL

$$= \frac{1}{3}\frac{a^3}{8} = \frac{a^3}{24}$$

$$= \frac{1}{3}a3a^2 - \frac{1}{3}a3aa + \frac{1}{3}aa^2 - \frac{1}{3}\frac{a}{2}3a^2 + \frac{1}{3}\frac{a}{2}3a\frac{a}{2} - \frac{1}{3}\frac{a}{2}\frac{a^2}{4}$$

$$= \underline{\underline{a^3}} - \underline{\underline{a^3}} + \frac{1}{3}a^3 - \frac{1}{2}a^3 + \frac{1}{4}a^3 - \underline{\underline{\frac{1}{24}a^3}}$$

$$= A^2 a^3 \Big[\underbrace{\frac{1}{3} - \frac{1}{2} + \frac{1}{4}}_{\frac{4-6+3}{12}} \Big] = A^2 a^3 \frac{1}{12} \quad \Rightarrow \quad \boxed{A = \sqrt{\frac{12}{a^3}}}$$

OR SIMPLY:

$$\langle \phi | \phi \rangle = 2 \cdot \int_0^{a/2} (Ax)^2 dx = 2A^2 \frac{a^3}{24} = A^2 \frac{a^3}{12} \overset{!}{=} 1$$

(2) HAMILTONIAN : $H = T + V$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \phi$$

$$E[\phi] = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} = -\langle\phi|\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|\phi\rangle \overset{\text{TRICK}}{=} \frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left|\frac{d\psi(x)}{dx}\right|^2 dx$$

$$= \frac{\hbar^2}{2m}\int_0^{a/2}\left|\frac{d}{dx}(Ax)\right|^2 dx + \frac{\hbar^2}{2m}\int_{a/2}^{a}\left|\frac{d}{dx}A(a-x)\right|^2 dx$$

$$= \frac{\hbar^2}{2m}\int_0^{a/2}|A|^2 dx + \frac{\hbar^2}{2m}\int_{a/2}^{a}|A(-1)|^2 dx = \frac{\hbar^2 A^2}{2m}\left\{\underbrace{[x]_0^{a/2}}_{a/2-\phi} + \underbrace{[x]_{a/2}^{a}}_{a-a/2}\right\}$$

$$= \frac{\hbar^2 A^2 a}{2m} \overset{\text{SUBSTITUTE } A}{=} \boxed{\frac{12\hbar^2}{2ma^2}} \quad \text{UPPER BOUND}$$

[DIFFERENT FROM METHOD IN GRIFFITHS]

COMPARE TO EXACT GROUND STATE ENERGY :

$$E_0 = \frac{\pi^2\hbar^2}{2ma^2} < E[\phi]$$

22% DIFFERENCE

SINCE $\pi^2 \simeq 9.86 < 12$

WITHOUT TRICK: $E[\phi] = \langle\phi|H|\phi\rangle = -\frac{\hbar^2}{2m}\int_0^{a/2}(Ax)\frac{d^2}{dx^2}(Ax)dx - \frac{\hbar^2}{2m}\int_{a/2}^{a}A(a-x)\frac{d^2}{dx^2}A(a-x)dx$

1ST DERIVATIVE GIVES A STEP FUNCTION, 2ND DERIVATIVE GIVES A DELTA FUNCTION; GRIFFITHS p. 297

EXAMPLE [THIS TIME WITH PARAMETER VARIATION]

REVIEW HARMONIC OSCILLATOR:

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

$$\omega = \sqrt{\frac{k}{m}} \quad ; \quad F = -kx$$

GROUND STATE

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

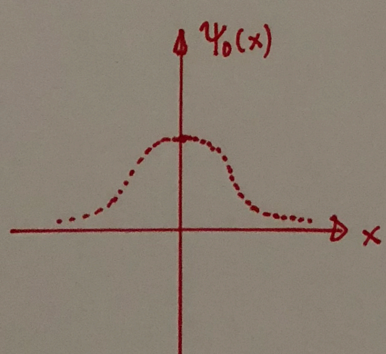
$$E_0 = \frac{1}{2}\hbar\omega$$

[EQS. 2.59/2.60 GRIFFITHS]

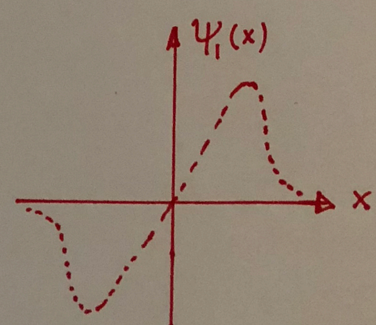
FIRST EXCITED STATE

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\, x\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_1 = \frac{3}{2}\hbar\omega$$



EVEN



ODD

ESTIMATE THE GROUND STATE ENERGY OF THE HARMONIC OSCILLATOR BY USING A TRIAL FUNCTION OF THE FORM

$$\phi_\alpha(x) = e^{-\alpha x^2} \quad , \; \alpha > 0$$

ADJUSTABLE PARAMETER

STEPS: (1) FIND NORMALIZATION $\langle \phi | \phi \rangle$

(2) CALCULATE $E[\phi] = \langle \phi | H | \phi \rangle$

(3) MINIMIZE $E[\phi]$

HELP: $\displaystyle\int_{-\infty}^{+\infty} dx\, e^{-bx^2} = \sqrt{\frac{\pi}{b}}$

[PROVIDE INTEGRAL →]

$$\int_{-\infty}^{+\infty} x^2 e^{-bx^2} dx = \frac{1}{2b}\sqrt{\frac{\pi}{b}}$$

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

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

DERIVATIVE : $\displaystyle \frac{d^2}{dx^2} e^{-\alpha x^2} = \frac{d}{dx}\left[-2\alpha x\, e^{-\alpha x^2} \right]$

$$= -2\alpha e^{-\alpha x^2} - 2\alpha x(-2\alpha x) e^{-\alpha x^2}$$

$$= -2\alpha e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2}$$

$$\langle \phi | H | \phi \rangle = \int_{-\infty}^{+\infty} dx\, e^{-\alpha x^2} \left[-\frac{\hbar^2}{2m}(-2\alpha e^{-\alpha x^2}) - \frac{\hbar^2}{2m}(4\alpha^2 x^2 e^{-\alpha x^2}) + \frac{m\omega^2}{2} x^2 e^{-\alpha x^2} \right]$$

$$= \int_{-\infty}^{+\infty} dx \left[\frac{\hbar^2 2\alpha}{2m} + \left(-\frac{\hbar^2 4\alpha^2}{2m} + \frac{m\omega^2}{2} \right) x^2 \right] e^{-2\alpha x^2}$$

$$= \underbrace{\int_{-\infty}^{+\infty} dx\, \frac{\hbar^2 2\alpha}{2m} e^{-2\alpha x^2}}_{\frac{\hbar^2 2\alpha}{2m}\sqrt{\frac{\pi}{2\alpha}}} + \left(-\frac{\hbar^2 4\alpha^2}{2m} + \frac{m\omega^2}{2} \right) \underbrace{\int_{-\infty}^{+\infty} x^2 e^{-2\alpha x^2} dx}_{\frac{1}{4\alpha}\sqrt{\frac{\pi}{2\alpha}}}$$

$$= \sqrt{\frac{\pi}{2\alpha}} \left[\frac{2\hbar^2\alpha}{2m} - \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha} \right]$$

$$= \sqrt{\frac{\pi}{2\alpha}} \left[\frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha} \right]$$

$$E[\phi] = \frac{\sqrt{\frac{\pi}{2\alpha}} \left[\frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha} \right]}{\sqrt{\frac{\pi}{2\alpha}}} = \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$$

$$\left[\int_{-\infty}^{+\infty} x^2 e^{-bx^2} dx = -\frac{\partial}{\partial b} \int_{-\infty}^{+\infty} e^{-bx^2} dx = -\frac{\partial}{\partial b} \left[\sqrt{\pi}\, b^{-1/2} \right] = \frac{1}{2}\sqrt{\pi}\, b^{-3/2} \right]$$

(3) $$\frac{d}{d\alpha} E[\phi] = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} \overset{!}{=} 0$$

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

$$\alpha^2 = \frac{m\omega^2 2m}{8\hbar^2} = \frac{m^2\omega^2}{4\hbar^2}$$

$$\alpha = \pm \frac{m\omega}{2\hbar}$$

RETAIN ONLY POSITIVE, PHYSICAL SOLUTION

OUR BEST ESTIMATE OF GROUND STATE ENERGY:

$$E_{min}[\phi] = \frac{\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{m\omega^2}{8\frac{m\omega}{2\hbar}} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \boxed{\frac{1}{2}\hbar\omega}$$

WE HAPPEN TO GET EXACTLY THE RIGHT GROUND STATE ENERGY (AND EIGENSTATE) BECAUSE THE FAMILY OF TRIAL FUNCTIONS WE CHOSE INCLUDES THE EXACT WAVE FUNCTION

$$\phi = \frac{1}{\left(\frac{\pi}{2\alpha}\right)^{1/4}} e^{-\alpha x^2} = \left(\frac{2m\omega}{2\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

WHAT ABOUT EXCITED STATES? [PROBLEM 7.4 IN GRIFFITHS]

IF WE CAN FIND A TRIAL FUNCTION, ϕ, THAT IS ORTHOGONAL TO THE EXACT GROUND STATE, ψ_0, THEN $E[\phi] \geq E_{\text{FIRST EXC. STATE}}$

PROOF: $|\phi\rangle = \sum_{n=0}^{\infty} c_n |\psi_n\rangle$ WITH $|\psi_0\rangle$ GROUND STATE

WE ASSUME $\langle \psi_0 | \phi \rangle = 0$

$$\Rightarrow \langle \psi_0 | \phi \rangle = \langle \psi_0 | \sum_{n=0}^{\infty} c_n \psi_n \rangle = \sum_{n=0}^{\infty} c_n \langle \psi_0 | \psi_n \rangle \overset{!}{=} 0$$

MEANING: $c_0 = 0$ [COEFFICIENT OF GROUND STATE IS ZERO]

$$\Rightarrow E[\phi] = \langle \phi | H | \phi \rangle = \sum_{n=1}^{\infty} E_n |c_n|^2 \geq \sum_{n=1}^{\infty} E_1 |c_n|^2 = E_1$$

SINCE $E_n \geq E_1$

(1) THIS SEEMS USELESS, SINCE WE DO NOT KNOW THE GROUND STATE BEFOREHAND;

HOWEVER, GIVEN A POTENTIAL WITH SOME SYMMETRY, WE MAY OFTEN PICK $\langle \psi_0 | \phi \rangle = 0$

EXAMPLE: IN 1D, IF POTENTIAL IS AN EVEN FUNCTION, THE GROUND STATE WAVE FUNCTION SHOULD ALSO BE EVEN; IF WE PICK AN ODD TRIAL FUNCTION, IT MUST BE ORTHOGONAL TO THE GROUND STATE

(2) YOU COULD TRY TO BE CLEVER:

IF YOUR GROUND STATE TRIAL FUNCTION GIVES A "CLOSE" RESULT FOR THE BINDING ENERGY, YOU COULD PICK A FIRST EXCITED STATE TRIAL FUNCTION THAT IS ORTHOGONAL TO THE GROUND STATE TRIAL FUNCTION;

BUT THEN THERE ARE TWO SOURCES OF UNCERTAINTY:

- GROUND STATE TRIAL FUNCTION IS NOT EXACT

  [FIRST EXCITED STATE TRIAL FUNCTION (MAY) (BE) (NOT) (ORTHOGONAL) TO EXACT GROUND STATE WAVE FUNCTION]

- FIRST EXCITED STATE ENERGY IS ONLY CALCULATED APPROXIMATELY

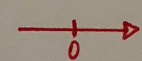
$\boxed{\text{EXAMPLE}}$ HARMONIC OSCILLATOR

CHOSE A TRIAL FUNCTION $\phi = x e^{-\alpha x^2}$ [ODD]

AND FIND AN ESTIMATE FOR THE ENERGY OF FIRST EXCITED STATE

SINCE TRIAL FUNCTION IS ODD, IT IS ORTHOGONAL TO (EVEN) GROUND STATE

$$\langle \psi_0 | \phi \rangle = \int_{-\infty}^{+\infty} dx \, \underbrace{\boxed{x e^{-\alpha x^2}}}_{\substack{\phi \\ \text{SIGN FLIP} \\ \text{AT } x=0}} \underbrace{\boxed{e^{-b x^2}}}_{\substack{\psi_0 \\ \text{EXACT}}} = 0$$



SKETCH SOLUTIONS:

[INTERMEDIATE STEPS NOT GIVEN]

$$E[\phi] = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{3\hbar^2}{2m} \alpha + \frac{3}{8} \frac{m \omega^2}{\alpha}$$

$$\frac{d}{d\alpha} E[\phi] = 0 \quad \text{YIELDS} \quad E[\phi] = \frac{3}{2} \hbar \omega$$

WHICH HAPPENS TO BE AGAIN THE EXACT SOLUTION BECAUSE OUR TRIAL FUNCTION HAS THE SAME SHAPE AS THE EXACT SOLUTION

$u(r) = r R(r)$

EXAMPLE

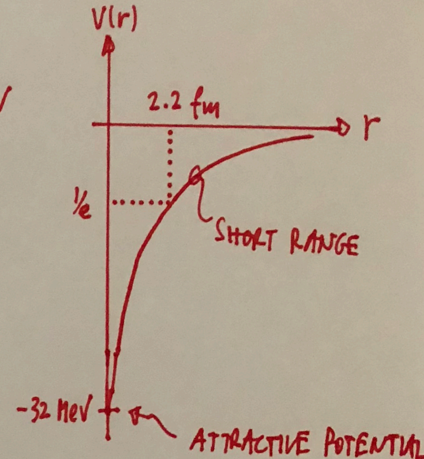
CALCULATE THE GROUND STATE BINDING ENERGY OF DEUTERIUM;

SLIDE ON DEUTERIUM

SUPPOSE THE STRONG NUCLEAR POTENTIAL IS GIVEN BY

$$V(r) = -A e^{-r/a}$$

WITH $a = 2.2$ fm AND $A = 32$ MeV



USE A TRIAL FUNCTION THAT BEHAVES SIMILARLY, i.e., A LARGE AMPLITUDE AT SMALL DISTANCE [NUCLEAR INTERIOR] AND A SHORT RANGE:

$$\phi(r) = R(r) = K e^{-\alpha r/2a}$$

NORMALIZATION

ADJUSTABLE PARAMETER

[PROVIDE INTEGRAL]

WE CAN ALSO ASSUME THAT THE GROUND STATE HAS ZERO ORBITAL ANGULAR MOMENTUM

- DEUTERON SPIN : 1^+
- MOSTLY $l = 0$ [S-STATE], WITH VERY SMALL D-STATE ADMIXTURE

FIND FIRST NORMALIZATION CONSTANT κ: [GROUP WORK: FIND κ^2]

$$\langle \phi | \phi \rangle = \langle RY | RY \rangle = \int_0^\infty dr\, r^2 \int_{4\pi} d\Omega\, |R(r)\, \underbrace{Y_\ell^m(\theta,\phi)}_{\text{NORMALIZED}}|^2$$

$$= \int_0^\infty dr\, r^2\, |R(r)|^2 \overset{!}{=} 1$$

$$\Rightarrow \int_0^\infty \kappa^2 e^{-\frac{\alpha r}{a}} r^2\, dr = \kappa^2 \underbrace{\left[\frac{e^{-\frac{\alpha}{a}x}\left(-\frac{\alpha}{a}x\left(\frac{\alpha}{a}x+2\right)-2\right)}{\left(\frac{\alpha}{a}\right)^3} \right]_0^\infty}_{\emptyset - \frac{(-2)}{\left(\frac{\alpha}{a}\right)^3}} = \kappa^2 \frac{2a^3}{\alpha^3} \overset{!}{=} 1$$

$$\boxed{\kappa^2 = \frac{\alpha^3}{2a^3}}$$

PROVIDE:

$$\int_0^\infty dx\, x^2 e^{-bx} = \left[\frac{e^{-bx}(-bx(bx+2)-2)}{b^3} \right]_0^\infty$$

FIND EXPECTATION VALUE $\langle \phi | H | \phi \rangle$

$$E[\phi] = \langle RY | H | RY \rangle = \int_0^\infty R H R \, r^2 dr \underbrace{\int_{4\pi} d\Omega \, |Y_0^0(\theta,\phi)|^2}_{=1}$$

$$= \int_0^\infty r^2 dr \, (\kappa e^{-\alpha r/2a}) \left(\frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V \right) (\kappa e^{-\alpha r/2a})$$

ZERO FOR GROUND STATE

$$= \kappa^2 \int_0^\infty r^2 dr \, (e^{-\alpha r/2a}) \left[-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r - A e^{-r/a} \right] (e^{-\alpha r/2a})$$

$$= \underbrace{-\frac{\hbar^2 \kappa^2}{2m} \int_0^\infty r^2 dr \, e^{-\alpha r/2a} \frac{1}{r} \frac{\partial^2}{\partial r^2} (r e^{-\alpha r/2a})}_{\mathrm{I}}$$

$$\underbrace{- A \kappa^2 \int_0^\infty r^2 dr \, e^{-\alpha r/2a} \, e^{-r/a} \, e^{-\alpha r/2a}}_{\mathrm{II}}$$

——— CONTINUE AS HOMEWORK ———→