For normalizable Solutions: $E > V_{min}$
Proof: TISE → $\psi'' = \frac{2m}{\hbar^2}(V_{(x)} - E)\psi$

Describes the state of a system

RELATIVISTIC → DIRAC EQUATION

Quantum Mechanics - Cheat Sheet:

The wave function $\Psi(\vec{x},t): \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$:

"Kinetic Term" "Potential" $h = 2\pi\hbar = 6{,}626 \cdot 10^{-34}$ [Js]

↳ Solution to Schrödinger equation: $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 \Psi + V(\vec{x},t)\Psi$ (NON-RELATIVISTIC)

↳ SE can be solved via Separation of Variables: $\Psi(\vec{x},t) = \psi(\vec{x})\varphi(t)$ (If Potential is only a function of $\vec{x}$)

→ $\varphi(t) = \exp\left(-i\frac{E_n}{\hbar}t\right)$ → TISE: $-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{x})\psi = E_n\psi$

(E_n ... Constant from Sep. of Var.)

↳ $\iiint |\Psi(\vec{x},t)|^2 dV = \iiint \Psi^* \Psi \, dV$ = Prob. of finding particle within V at time t

↳ NORMALIZATION: $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi|^2 dz\,dy\,dx \overset{!}{=} 1$ → "Particle has to be somewhere"
If normalized at time t = 0 → Stays normalized

↳ Position Space: $\Psi(\vec{x},t) = \hbar^{\frac{3}{2}}(2\pi)^{-\frac{3}{2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Phi(\vec{p},t)\, e^{\frac{i}{\hbar}(xp_x + yp_y + zp_z)} d\vec{p}$

↳ Momentum Space: $\Phi(\vec{x},t) = (2\pi\hbar)^{-\frac{3}{2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi(\vec{x},t)\, e^{-\frac{i}{\hbar}(xp_x + yp_y + zp_z)} dx\,dy\,dz$

(Probabilities, that particle moving ... momentum between p_1 & p_2: $\int_{p_1}^{p_2} |\Phi|^2 dp$)

↳ Standard BC for $\psi(x)$: → $\psi(x)$ is always continous
→ $\frac{d}{dx}\psi(x)$ is continous (except at points where $V \to \infty$)

Then if $V(x) = -\alpha\delta(x)$: $\Delta\left(\frac{d\psi}{dx}\right)\Big|_{x=0} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)dx = -\frac{2m\alpha}{\hbar^2}\psi(0)$

Statistic Review: $\rho(x)$ ... Probability density

→ $P_{x\in[a;b]} = \int_a^b \rho(x)\,dx$

→ $\langle x \rangle = \int_{-\infty}^{\infty} x\rho(x)\,dx$ .... Mean Value

→ $\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)\rho(x)\,dx$ → $\langle x^2\rangle \geq \langle x\rangle^2$

→ $\sigma^2 = \langle(x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$

(Average deviation from $\langle x\rangle$)

Properties of Separable Solutions:

i) Stationary States: $\frac{d}{dt}\langle Q\rangle = 0, \forall Q$

ii) Definite Total Energy: $\langle H\rangle = E$ & $\sigma_H = 0$

iii) Form a complete Set: $\Psi_{GENERAL} = \sum c_n \Psi_{SOL}^{SEP}$

iv) Ψ_n's are STANDING WAVES (with multiple momenta)

Dirac Notation:

↳ Ψ's live in Hilbert Space (L_2-Space)

↳ $|\Psi\rangle = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$ .... Ket

↳ $\langle\Psi| = (c_1^*, ..., c_n^*)$ .... Bra

→ INNER PRODUCT: $\langle f|g\rangle = \int f^* g\,dx$ (Integrate over whole space where f, g are defined)

ORTHOGONALITY: $\langle f|g\rangle = 0$

ORTONORMALITY: $\langle\Psi_n|\Psi_m\rangle = \delta_{nm}$

Commutators: $[\hat{x}, \hat{p}] = i\hbar$

CALCULATE: Use a test-function (that will be dropped afterwards)

↳ Two operator $\hat{A}, \hat{B}$, their commutator is $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

↳ $[\hat{A}\hat{B}, \hat{C} + \hat{D}] = [\hat{A}\hat{B}, \hat{C}] + [\hat{A}\hat{B}, \hat{D}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} + [\hat{A}\hat{B},\hat{D}]$

Generalized Statistical Interpretation & Observables:

↳ Observables Q are represented by a linear, hermitian operator $\hat{Q}$! ($\hat{Q} = f(\hat{x},\hat{p})\ \forall \hat{Q}$)
(Since the expectation value $\langle Q\rangle$ must be real)

↳ HERMITIAN: $\langle\Psi|\hat{Q}\Psi\rangle = \langle\hat{Q}\Psi|\Psi\rangle$ (Usually it would be $\langle f|g\rangle = (\langle g|f\rangle)^*$)

(COMMUTATOR of HERMITIAN operators is ANTI-HERMITIAN, i.e.: $\hat{Q}^\dagger = (\hat{Q}^T)^* = -\hat{Q}$)

↳ Measurement an observable Q is certain to give Eigenvalue of $\hat{Q}$

↳ The probability for each Eigenvalue $q^{(n)}$ depends on the corresponding Eigenfunction f_n

SPECTRA: (Collection of all Eigenvalues)

i) DISCRETE Spectrum: Prob. of finding particle in State f_n (giving $q^{(n)}$ when measure) is $|c_n|^2$, where $c_n = \langle f_n|\Psi\rangle$ (ORTHO-NORMALIZE)

ii) CONTINOUS Spectrum: Prob. of finding particle in range dz is $|c(z)|^2 dz$, where $c(z) = \langle f_z|\Psi\rangle$ (CANNOT BE NORMALIZED)
(That is: Returning Eigen-value $q(z)$, when measured)

↳ Determinate States: (≙ Measurement on Q gives deterministic value q)
CAN BE NORMALIZED IFF particle state = Eigenfunction of $\hat{Q}$: $\hat{Q}\Psi = q\Psi$ → REAL

DISCRETE SPECTRA:	CONTINOUS SPECTRA:
i) Eigenvalues are real ii) Eigenfunctions bel. to diff EV → orthogonal iii) Eigenfunc. → complete	i) Restrict to real Eigenvalues $q(z)$ ii) Then Eigenfunc are Dirac-ORTHONORM.: $\langle f_{z_1}|f_{z_2}\rangle = \delta(z_1 - z_2)$ (Cont. Variable)

EXAMPLES of CONTINOUS SPECTRA:

MOMENTUM:
i) Eigenequation: $-i\hbar \frac{\partial}{\partial x} f_p(x) = p f_p(x)$
ii) Restrict $p \in \mathbb{R}$: Eigenfunc.: $f_p = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$ → De Broglie
iii) Dirac orthogonal: $\langle f_{p'} | f_p \rangle = \delta(p-p')$
Eigenfunc. are sinusoidal with $\lambda = \frac{2\pi\hbar}{p}$

POSITION:
i) Eigenequation: $\hat{x} g_\lambda(x) = \lambda g_\lambda(x)$
ii) Eigenfunc.: $g_\lambda(x) = A\,\delta(x-\lambda)$
iii) Again → Dirac Orthogonal

$[\hat{x}^2, \hat{p}^2] = 2i\hbar \langle \hat{x}\hat{p}+\hat{p}\hat{x} \rangle$

ad Observables:
↳ $\hat{x} = x$, $\hat{\vec{x}} = \vec{x}$ ↳ $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$, $\hat{\vec{p}} = -i\hbar \vec{\nabla}$ ↳ $\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})$

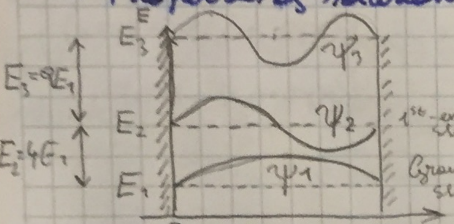
↳ $\langle Q(x,p) \rangle = \langle \Psi | \hat{Q}(\hat{x},\hat{p}) \Psi \rangle$ WHY SANDWICH? Because in the derivation for $\hat{p}$, we saw the derivative only acts upon 2nd Ψ

↳ Ehrenfest's Theorem: Expectation values obey classical laws! ($\langle T \rangle = \frac{1}{2m}\langle p^2 \rangle$) ← Kin. Energy

The infinite Square-Well: $V(x) = \begin{cases} 0, & x \in [0;a] \\ \infty, & \text{else} \end{cases}$

↳ $\psi^n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a}x)$ ↳ $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ ↳ $n = 1, 2, 3, \dots$

↳ Properties of solutions: i) Even / Odd (alternately) w.r.t. center of well
ii) n-th solution → n-1 Nodes
iii) Mutually orthogonal: $\langle \psi^n | \psi^m \rangle = \delta_{nm}$
iv) ψ^n's are complete → $\sum |c_n|^2 \overset{!}{=} 1$



$\langle H \rangle = \sum_{i=1}^{\infty} |c_n|^2 E_n$, $\langle H \rangle > 0$

↳ Given $\Psi(x,0)$: i) $\Psi(x,0) \overset{!}{=} \sum_{n=1}^{\infty} c_n \psi^n(x)$ → $c_n = \sqrt{\frac{2}{a}} \int_0^a \sin(\frac{n\pi}{a}x) \Psi(x,0)\, dx$
NORMALIZE
ii) $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi^n(x) \exp(-i\frac{E_n}{\hbar}t)$, $|c_n|^2$ ... Prob. of measuring energy E_n

The Harmonic Oscillator: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$, where $\omega = \sqrt{\frac{k}{m}}$

Solution to ODE: $\hat{a}_-\psi_0 = 0$

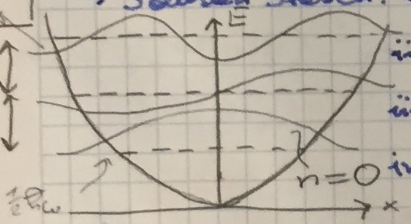
↳ $\psi_0 = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}} \exp(-\frac{m\omega}{2\hbar}x^2)$, $E_0 = \frac{1}{2}\hbar\omega$ (Plug ψ_0 into TISE)
→ where $\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x)$ (Raising Operator / Lowering Operator)

↳ $\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n \psi_0$, $E_n = (\frac{1}{2}+n)\hbar\omega$

↳ $\hat{a}_+\psi_n = \sqrt{n+1}\,\psi_{n+1}$ ↳ $\hat{a}_-\psi_n = \sqrt{n}\,\psi_{n-1}$ $\langle x \rangle_n = \langle p \rangle_n = 0 \;\forall n$

↳ Solution Sketch: i) $\hat{a}_\pm \hat{a}_\mp = \frac{1}{\hbar\omega}\hat{H} \mp \frac{1}{2}$ ⇒ $\hat{H} = \hbar\omega(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2})$, since $[\hat{a}_+, \hat{a}_-] = 1$
ii) TISE: $\hbar\omega(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2})\psi = E\psi$ → We FACTORED $\hat{H}$
iii) If ψ satisfies TISE, so does $\hat{a}_\pm\psi$, with $(E \pm \hbar\omega)$: $\hat{H}(\hat{a}_\pm\psi) = (E \pm \hbar\omega)(\hat{a}_\pm\psi)$
iv) Apply $\hat{a}_-$ repeatedly → At some point energy gets too low! ($E > V_{min} = 0$) $\hat{a}_-\psi_0$ → not normalizable (Either $\hat{a}_-\psi_0 = 0$ or $\lim_{x\to\infty} \hat{a}_-\psi_0 \neq 0$) Cannot explain why these

TUNNELING: Negative kinetic energy



The free particle: $V = 0$

$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-)$
$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-)$

↳ Separable (≙ stationary) Sol.: $\Psi^k(x,t) = A\exp(i[kx - \frac{\hbar k^2}{2m}t])$
$k = \pm\frac{\sqrt{2mE}}{\hbar}$, with $k \begin{cases} > 0 \Rightarrow \text{wave travelling to right} \\ < 0 \Rightarrow \text{wave travelling to left} \end{cases}$

E = CONTINOUS and so is k → $\int dk$

↳ $\Psi^k(x,t)$ NOT NORMALIZABLE → No free particle with definite energy!

↳ Still Ψ^k complete ⇒ $\Psi^{GEN} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k) \exp(i[kx - \frac{\hbar k^2}{2m}t])\, dk$

↳ $\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)\exp(ikx)\,dk \Leftrightarrow g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)\exp(-ikx)\,dx$ $g(k)$ ... SHAPE FUNCTION
MAY DEPEND ON STATE — PLANCHEREL'S THEOREM

The Uncertainty-Principle: GUP

↳ $\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$ (Since $\hat{A}, \hat{B}$ → Hermitian: $\langle[\hat{A},\hat{B}]\rangle$ is purely imaginary → see Commut.)

BOUND STATE: $E < (V(-\infty) \,\&\&\, V(+\infty))$
SCATTERING STATE: $E > (V(-\infty) \,||\, V(+\infty))$

↳ Incompatible Observables → $[\hat{A},\hat{B}] \neq 0$ $\sigma_x^2\sigma_p^2 \geq (\frac{\hbar}{2})^2$

↳ Compatible Observables → $[\hat{A},\hat{B}] = 0$ → Share the same Eigenbasis!

↳ Energy-Time-Uncertainty: $\Delta t \Delta E \geq \frac{\hbar}{2}$ (depending on observable we look at) ← To derive we used GUP

IT FOLLOWS: If $[\hat{H},\hat{Q}] = 0$ the quantity is CONSERVED

→ Δt .... Amount of time it takes the expectation value of Q to change by one standard deviation: $\Delta t = \frac{\sigma_Q}{\left|\frac{d\langle Q \rangle}{dt}\right|}$, where $\frac{d\langle Q \rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial \hat{Q}}{\partial t}\rangle$

Fails of course if $\left|\frac{d\langle Q \rangle}{dt}\right| = 0$, division by 0

→ ΔE ... σ_H

Radius $r \in [0;\infty]$
Azimuthal $\varphi \in [0;2\pi]$
Polar A. $\vartheta \in [0;\pi]$
$\rightarrow dV = r^2 \sin\vartheta \, dr \, d\vartheta \, d\varphi$

Term in $[\cdot] = \vec{\nabla}^2 \psi$

TISE in Spherical Coord.: $-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\psi + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}\psi\right) + \frac{1}{r^2\sin^2\vartheta}\left(\frac{\partial^2}{\partial\varphi^2}\psi\right)\right] + V\psi = E\psi$

↳ Assuming $V = V(r)$ (Radially symmetric) → Sep. of Var.: $\psi = R(r) Y(\vartheta,\varphi) = \frac{u(r)}{r} Y(\vartheta,\varphi)$

Constant of Sep. of Var. $= l(l+1)$

i) Radial equation: $-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$ — "Centrifugal term"

ii) Angular equation: $\frac{1}{Y}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}Y\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}Y\right] = -l(l+1)$

→ Occurs when solving Laplace Equ. in Electrodyn.

Angular Equation:

↳ Sep. of Var.: $Y(\vartheta,\varphi) = \Theta(\vartheta)\Phi(\varphi)$ ⇒ Constant m_l^2 ⇒ Leads to

i) $\frac{1}{\Theta}\left[\sin\vartheta\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d}{d\vartheta}\Theta\right)\right] + l(l+1)\sin^2\vartheta = m_l^2$

ii) $\frac{d^2}{(d\varphi)^2}\Phi = -m_l^2\Phi \Rightarrow \boxed{\Phi(\varphi) = e^{\pm i m_l \varphi}}$ BC.: $\Phi(\varphi+2\pi) = \Phi(\varphi) \Rightarrow m_l = 0, \pm 1, \pm 2, \ldots$

If we said $\varphi - 2\pi$: $m_l = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$

↳ Solution to i): $\boxed{\Theta(\vartheta) = A P_l^m(\cos\vartheta)}$, where $P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$ (Legendre Polynomial) (Rodrigues Formula)

$P_l^m(x) = (1-x^2)^{\frac{|m|}{2}}\left(\frac{d}{dx}\right)^{|m|} P_l(x)$ (Legendre function)

↳ For $|m| > l \rightarrow P_l^m = 0$ & For P_l: $l \in \mathbb{N}$

So: $l = \{0,1,2,\ldots\}$ (Azimuthal Quantum Number) $m_l = \{-l, -l+1, \ldots, l-1, l\}$ (Magnetic Quantum Number)

For given l, there are $2l+1$ values so that $P_l^m \neq 0$

↳ Normalizing separately: $\int_0^\infty |R(r)|^2 r^2 \, dr \stackrel{!}{=} 1$ $\int_0^{2\pi}\int_0^\pi |Y|^2 \sin\vartheta \, d\vartheta \, d\varphi \stackrel{!}{=} 1$

NOTE: There should be 2 linear indep. sol. to Θ-equ. but they blow up

Yields SPHERICAL HARMONICS: $\boxed{Y_l^m = (-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\varphi}P_l^m(\cos\vartheta)}$

ORTHONORM. of Y_l^m: $\int_0^{2\pi}\int_0^\pi (Y_l^m)^*(Y_{l'}^{m'})\sin\vartheta \, d\vartheta \, d\varphi = \delta_{ll'}\delta_{mm'}$ (Because they are eigenfunc. to Hermitian operator)

The Hydrogen Atom:

↳ $V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$ (For hydrogenic atoms, i.e. nucleus with Z protons (Ze) but only 1 electron → Substitute $\tilde{e} = \sqrt{Z}e$; $V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r} \rightarrow \frac{-\tilde{e}^2}{4\pi\varepsilon_0 r}$! Same Subst. in results!)

↳ Solution Sketch:

i) Peel off asymptotic behaviour (i.e. sol. for $u \rightarrow 0$ & $u \rightarrow \infty$)

ii) Suggests Subst.: $u(r) = (\kappa r)^{l+1} e^{-\kappa r} v(r)$, $\kappa = \frac{\sqrt{-2mE}}{\hbar}$

iii) Express $v(r)$ as power series → Plug in → Compare Coeff.!

We obtain a recursion formula for coeff. c_j! Sol. would blow up for large $j \rightarrow j_{max}$ → Series terminates! Here comes the principal Quantum number n!!!

$R(r)$... Radial wave function ≠ Radial probability distribution
RADIAL PROB. DENSITY/DISTR.
$P(r) = \int_0^{2\pi}\int_0^\pi |\psi|^2 r^2 \sin\vartheta \, d\vartheta \, d\varphi$

↳ Solution: i) $E_n = -\left(\frac{m}{2\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0}\right]^2\right)\frac{1}{n^2} = \frac{E_1}{n^2} = -\frac{13.6}{n^2}eV$, $n = 1,2,3$

ii) $R_{nl}(r) = \sqrt{\left(\frac{2}{na}\right)^3\frac{(n-l-1)!}{2n[(n+l)!]^3}}\exp\left(-\frac{r}{na}\right)\left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)$

DEGENERACY of n^{th} energy level is n^2! n^{th}-shell can hold $2n^2$ electrons (Since $\sum_0^{n-1}(2l+1) = n^2$)

where the Bohr-Radius is: $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529$ Å

L_{q-p}^p ≙ Laguerre Polynomial → FORMULA makes sense ONLY for $l = 0,1,2,\ldots,n-1$

↳ Can only absorb/emit discrete values of energy, i.e. $|E_{n'} - E_n|$

↳ Wavelength of emitted light (when electron goes from n_i to n_f): $\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$R = \frac{m}{4\pi c\hbar^3}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$ $[m^{-1}]$

SPHERICAL COORD.:
$L_x = i\hbar(\sin\varphi\frac{\partial}{\partial\vartheta} + \cos\varphi\cot\vartheta\frac{\partial}{\partial\varphi})$
$L_y = i\hbar(-\cos\varphi\frac{\partial}{\partial\vartheta} + \sin\varphi\cot\vartheta\frac{\partial}{\partial\varphi})$
$L_z = -i\hbar\frac{\partial}{\partial\varphi}$

UV: $n_f = 1$... Lyman
visible: $n_f = 2$... Balmer
Infrared: $n_f = 3$... Paschen

Orbital Angular Momentum:

↳ $\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}} = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \hat{x}\hat{p}_y - \hat{y}\hat{p}_x)$

Also $[\hat{H}, L^2] = [\hat{H}, L_z] = 0$ Because they share the same eigenfunctions

↳ $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$, $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$, $[L^2, \vec{L}] = 0$

↳ To determine Eigenvalues/-func. (of L^2 & L_z) we define: $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$, $[L_z, L_\pm] = \pm\hbar L_\pm$, $[L^2, L_\pm] = 0$

→ z-direction randomly chosen!

↳ $L^2 f = \lambda f$ & $L_z f = \mu f$ ⇒ $L^2(L_\pm f) = \lambda(L_\pm f)$ & $L_z(L_\pm f) = (\mu \pm \hbar)(L_\pm f)$

$L_\pm f_l^m = A_l^m f_l^{m\pm1}$ where $A_l^m = \hbar\sqrt{l(l+1) - m(m\pm1)}$

↳ $L_\pm$ increases/decreases z-component of angular momentum but keeps total length unchanged → at some top/bottom rung f has to become unphysical (i.e. not normalizable: Either $L_\pm f_{\text{BOTTOM}}^{\text{TOP/}} = 0$ or $\lim_{x\to\infty} L_\pm f_n^{T/} \neq 0$)

← Again choose this one! Why? DUNNO

ADDITION of angular momentum:

$\hat{J} = \hat{J}_1 + \hat{J}_2$: New angular momentum vector lives in $\otimes$-Vector Space of old ones

$|j_1| + |j_2| = \{ j_1 + j_2, (j_1+j_2)-1, \dots, |j_2 - j_1| \}$

HUND'S RULES:

I: Largest S most stable

II: Fixed S → Largest L most stable

III: Fixed S&L: i) Subshell less than half full: Smaller J is most stable

ii) Subshell more than half full: Largest J is most stable

Where $\mu_{TOP} = l\hbar$, $\mu_{BOTTOM} = \bar{l}\hbar$

Orbital Angular Momentum:

↳ $L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z \Rightarrow \begin{cases} \text{Top Rung}: \lambda = \hbar^2 l(l+1) \\ \text{Bottom Rung}: \lambda = \hbar^2 \bar{l}(\bar{l}-1) \end{cases} \Rightarrow l = -\bar{l}$

↳ Finally: $L^2 f_l^m = \hbar^2 l(l+1) f_l^m$ & $L_z f_l^m = \hbar m f_l^m$, $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$; $m = -l, -l+1, \dots, l-1, l$

↳ Angular momentum is a CONE! (never aligned with z-axis)

↳ Eigenfunctions: $f_l^m = Y_l^m$ $\left(L^2 = -\hbar^2 \left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} \right],\ L_z = -i\hbar\frac{\partial}{\partial\varphi} \right)$ ‖ Same system of equ. as angular equ. when plugged into Eigenequations

Spin Angular Momentum:

↳ Particle acts AS IF it was spinning! (Spin comes from Relativistic QM → we will base the following on experiments & Axioms)

↳ AXIOMS: $[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$, $[\hat{S}_y, \hat{S}_z] = i\hbar \hat{S}_x$, $[\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$, $[\hat{S}^2, \hat{S}] = 0$

$s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ $\hat{S}^2 |s\ m_s\rangle = \hbar^2 s(s+1) |s\ m_s\rangle$; $\hat{S}_z |s\ m_s\rangle = \hbar m_s |s\ m_s\rangle$

$m_s = -s, -s+1, \dots, s-1, s$ $\hat{S}_\pm |s\ m_s\rangle = \hbar\sqrt{s(s+1) - m(m\pm1)}\, |s\ (m\pm1)\rangle$, $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ ← NOT observable

↳ SPIN-QN s is fixed for each particle (Pi-Meson: $s=0$, Electrons $s=\frac{1}{2}$; Photons: $s=1$, Deltas $s=\frac{3}{2}$; Gravitons: $s=2$)

Spin ½:

NORMALIZE!!!

↳ Choose the Eigenbasis of $\hat{S}_z$ to describe the general Spin State (represented by a Spinor). $|\chi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} = a|\tfrac{1}{2}\ \tfrac{1}{2}\rangle + b|\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle = a\uparrow + b\downarrow$

↳ In this Basis: $\hat{S}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\hat{S}_x = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\sigma_x}$, $\hat{S}_y = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\sigma_y}$, $\hat{S}_z = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\sigma_z}$ ← PAULI-MATRICES

IF WE CHOOSE A DIFFERENT BASIS: Do Similarity Transformation

DERIVE USING: (*) In a different basis, S_+/S_- can be obtained from the eigenequation! (i.e. row-per eigenvalue) AXIOM

$S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ ‖ $S_x = \frac{1}{2}(S_+ + S_-)$, $S_y = \frac{1}{2i}(S_+ - S_-)$

2-Particle-Systems:

↳ Ψ becomes a function of both position vectors: $\Psi(t, \vec{r}_1, \vec{r}_2)$

↳ The Hamiltonian is $\hat{H} = \underbrace{-\frac{\hbar^2}{2m_1}\nabla_1^2}_{\text{KIN. EN. of \#1}} \underbrace{- \frac{\hbar^2}{2m_2}\nabla_2^2}_{\text{KIN. EN. of \#2}} + \hat{V}(\vec{r}_1, \vec{r}_2)$ → INCLUDING INTERACTION

↳ Prob. of finding Part. #1 in volume d^3r_1 AND particle #2 in d^3r_2 is $|\Psi(t, \vec{r}_1, \vec{r}_2)|^2 d^3r_1 d^3r_2$

TISE: $\left[-\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2m_r}\nabla_r^2 + V(r)\right]\psi = E\psi$

↳ Problem becomes separable if: $\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$ … Centre of mass; $M = m_1 + m_2$ Total Mass

$\vec{r} = \vec{r}_1 - \vec{r}_2$ … Relative motion; $m_r = \frac{m_1 m_2}{m_1 + m_2}$ Reduced Mass

INTERACTION POTENTIAL for 2-Particle System: $V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\vec{r}|}$

Atoms:

$n = 1, 2, 3$ # Nodes (Rad. + Plane)

$l = 0, 1, \dots, n-1$ # Planar Nodes

$m_l = -l, -l+1, \dots, l-1, l$

↳ Z… Atomic number → Charge of nucleus $= Ze \Rightarrow$ Z electrons

↳ $\hat{H} = \sum_{j=1}^{Z}\left[\left\{\underbrace{-\frac{\hbar^2}{2m}\nabla_j^2}_{j\text{th kinetic energy}} \underbrace{- \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_j}}_{j\text{th interaction with nucleus}}\right\} + \frac{1}{2}\left(\frac{1}{4\pi\epsilon_0}\right)\sum_{j\neq k}^{Z}\frac{e^2}{|\vec{r}_j - \vec{r}_k|}\right]$ → Since we are "double counting"; DEVIL'S TERM: Repulsive Interaction between electrons j&k

SINGLET STATE: $\chi^{OVER}_{ALL} = \frac{\sqrt{2}}{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

↳ 1st-approx.: We cancel the Interaction Term! → Electrons are in single particle hydrogenic states → #1: $\Psi_{n_1 l_1 m_1}$, #2: $\Psi_{n_2 l_2 m_2}$

$\Psi_a \neq \Psi_b$: $C = \frac{1}{\sqrt{2}}$; $\Psi_a = \Psi_b$: $C = \frac{1}{2}$

↳ How to combine? i) Distinguishable: $\Psi^{OVER}_{ALL} = \Psi_a(\vec{r}_1)\cdot\Psi_b(\vec{r}_2)$ ↳ Different mass / charge …

How to choose sign? ii) Indistinguishable: $\Psi^{OVER}_{ALL} = C[\Psi_a(\vec{r}_1)\Psi_b(\vec{r}_2) \pm \Psi_b(\vec{r}_1)\Psi_a(\vec{r}_2)]$ (Electrons)

Proof: Relativistic QM

↳ AXIOM: $\Psi^{OVER}_{ALL} = \Psi^{SPATIAL}\cdot|\chi\rangle$ = symmetric (antisymmetric) for Bosons (Fermions) with respect to exchange of $\vec{r}_1$ & $\vec{r}_2$ ($s = 1, 2, \dots$; $s = \frac{1}{2}, \frac{3}{2}, \dots$)

↳ Exchange Operator: $\hat{P}\Psi(\vec{r}_1, \vec{r}_2) = \pm\Psi(\vec{r}_2, \vec{r}_1)$, $[\hat{P}, \hat{H}] = 0$ ↳ Conserved → Symmetry does not change with time

↳ PAULI-EXLUSION PRINCIPLE: 2 Fermions cannot have same set of (n, l, m_l, m_s)

SCREENING: e^--e^--Interaction screen outer shell ($\uparrow r$) from charge of nucleus: $E\uparrow$

i) Symmetric wavefunction: Tend to locate particles close together

ii) Antisymmetric wavefunction: Tend to locate particles far apart

$\langle(x_1 - x_2)^2\rangle = \langle x^2\rangle_a + \langle x^2\rangle_b - 2\langle x\rangle_a\langle x\rangle_b \mp 2|\langle x\rangle_{ab}|^2$

$\langle x\rangle_{ab} = \langle a|x|b\rangle$

Term Symbol: $^{2S+1}L_J$

Z, El	Ground State
1 H	$^2S_{1/2}$
2 He	$^1S_0$
3 Li	$^2S_{1/2}$
4 Be	$^1S_0$
5 B	$^2P_{1/2}$
6 C	$^3P_0$
7 N	$^4S_{3/2}$
8 O	$^3P_2$
9 F	$^2P_{3/2}$
10 Ne	$^1S_0$
11 Na	$^2S_{1/2}$
12 Mg	$^1S_0$
13 Al	$^2P_{1/2}$
14 Si	$^3P_0$
15 P	$^4S_{3/2}$
16 S	$^3P_2$
17 Cl	$^2P_{3/2}$
18 Ar	$^1S_0$
19 K	$^2S_{1/2}$
20 Ca	$^1S_0$
21 Sc	$^2D_{3/2}$
22 Ti	$^3F_2$
23 V	$^4F_{3/2}$
24 Cr (EXCEPT)	$^7S_3$
25 Mn	$^6S_{5/2}$
26 Fe	$^5D_4$
27 Co	$^4F_{9/2}$
28 Ni	$^3F_4$
29 Cu (EXCEPT)	$^2S_{1/2}$
30 Zn	$^1S_0$
31 Ga	$^2P_{1/2}$
32 Ge	$^3P_0$
33 As	$^4S_{3/2}$
34 Se	$^3P_2$
35 Br	$^2P_{3/2}$
36 Kr	$^1S_0$

At room temperature $E = k_B T \gg \Delta E$ (for large n)

TOTAL ENERGY OF A FERMI-GAS:
(= free electron gas)

$dE = \frac{\hbar^2 k^2}{2m} \cdot \frac{V}{\pi^2} k^2 dk$

$E_{TOT} = \frac{\hbar^2 V}{2\pi^2 m} \int_0^{k_F} k^4 dk$

In k-space: Shell of thickness dk has Volume $V_{SHELL} = \frac{1}{8}(4\pi k^2)dk$

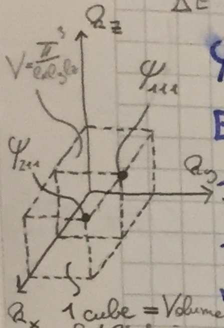
e^- in shell $= \frac{2 \cdot V_{SHELL}}{V_{STATE}} = \frac{2 \cdot (\frac{1}{2}\pi k^2)}{\frac{\pi^3}{V}} = \frac{V}{\pi^2} k^2 dk$

Each e^- carries $E_k = \hbar^2 k^2/(2m)$

Solids:

↳ 1st - model: "free electron gas" (i.e.: valence electrons) doesn't feel any forces from nuclei; only from (or from e^--interaction) walls → Particles in a box: $V = \begin{cases} 0, & x \in [0; l_x], y \in [0; l_y], z \in [0, l_z] \\ \infty & \text{else} \end{cases}$

For large n: (usual case) $\Delta E \ll 1$ → Energy bands



$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{l_x l_y l_z}} \sin(\frac{n_x \pi}{l_x} x) \sin(\frac{n_y \pi}{l_y} y) \sin(\frac{n_z \pi}{l_z} z)$, QN: $n_x, n_y, n_z = 1, 2, \dots$

$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m}\left[(\frac{n_x}{l_x})^2 + (\frac{n_y}{l_y})^2 + (\frac{n_z}{l_z})^2\right] = \frac{\hbar^2}{2m}|\vec{k}|^2$, where $\vec{k} = \left(\frac{n_x \pi}{l_x}, \frac{n_y \pi}{l_y}, \frac{n_z \pi}{l_z}\right)$

In k-space states with same energy occupy the surface of a sphere (radius $|\vec{k}|$)

Highest occupied energy level: Fermi-Energy with corresponding radius in k-space k_F

"Total volume in $\vec{k}$-space" $= \frac{1}{2} \cdot$ (# e^-) $\cdot$ ("Volume occupied in $\vec{k}$-space per State")

(only valid for # $e^- \gg 1$ -> Cubes are "pixels")

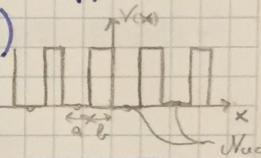
$\frac{1}{8}(\frac{4}{3}\pi k_F^3) = \frac{1}{2}(N q)(\frac{\pi^3}{l_x l_y l_z}) = \frac{1}{2} \rho \pi^2$, ρ... "free electron density"

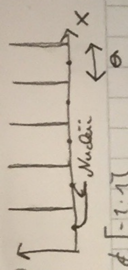
(# atoms; # valence e^-/atom; Total volume of solid)

FERMI-ENERGY: $E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m}(3\rho\pi^2)^{\frac{2}{3}}$, $\rho = \frac{Nq}{l_x l_y l_z} = \frac{Nq}{V}$

Density of states: For arbitrary Energy -> $Nq = \frac{V}{3\pi^2}(\frac{2mE}{\hbar^2})^{3/2} \Rightarrow D(E) = \frac{\partial(Nq)}{\partial E}$

1-electron levels per interval $[E, E+dE]$ $\quad D(E) = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\sqrt{E}$ (3D - case)





↳ 2^{nd} - model: Dirac-Comb (Derived from Kronig-Penney)

$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$ (a: Lattice - constant)

Solution in 1st-cell: $\psi(x) = A\sin(kx) + B\cos(kx)$, $x \in [0; a]$

Sol. in cell left from orig: $\psi(x) = e^{-iKa}(A\sin([x+a]k) + B\cos([x+a]k))$, $x \in [-a; 0]$ (via Bloch's-Theorem)

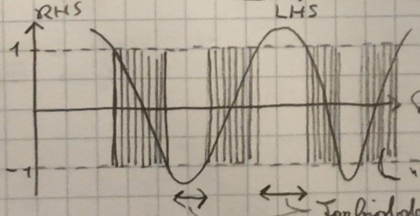
BC: i) $\psi_{(0)} \to B = e^{-iKa}(A\sin(ka) + B\cos(ka))$

ii) $\psi'_{(0)} \to kA - e^{-iKa}k(A\cos(ka) - B\sin(ka)) = \frac{2m\alpha}{\hbar^2}B$

Combine: $\underbrace{\cos Ka}_{LHS} = \underbrace{\cos ka + \frac{m\alpha}{\hbar^2 k}\sin(ka)}_{RHS}$

Since $\cos(Ka) \in [-1, 1]$ the equation cannot be solved for RHS $\notin [-1, 1]$

Only using we calculated probability $|\psi_{(x)}|^2 = |\psi|^2$ Bloch's Theorem → Solutions → NOW → Bands



Solutions for (ka) → bands
Therefore: Energies are bands
$E = \frac{\hbar^2 k^2}{2m}$

BLOCH's - Theorem:

For a periodic potential (i.e. $V(x+a) = V(x)$) the wave function satisfies $\psi(x+a) = e^{iKa}\psi(x)$, $K \in \mathbb{R}$ ($K = k$ else, $K \neq k(x)$)

Proof: "Displacement Op." $\hat{D}f(x) = f(x+a)$

$[\hat{D}, \hat{H}] = 0$ (since $\frac{d}{dx}(x+a) = 1$)

$\hat{D}$ & $\hat{H}$ share the same Eigenfunc.

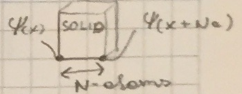
We can write for wave-func. $\hat{D}\psi(x) = \psi(x+a) = \lambda\psi(x) = e^{iKa}\psi$

Why $K \in \mathbb{R}$? -> Impose boundary cond. (Wrapping x-axis in a circle!!!)

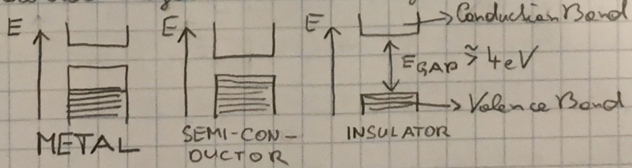
$\psi(x+Na) = \psi(x) \Rightarrow e^{iNKa}\psi(x) = \psi(x)$

$K = \frac{2\pi}{Na} n$ $(n = 0, \pm 1, \pm 2, \dots)$

(We write $e^{i\dots}$ just different way)

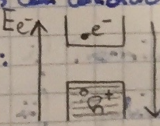


↳ Classification:



↳ Conductivity: To conduct -> e^- move -> kinetic energy -> e^- need empty states just above in energy -> Partially filled bands can conduct, filled bands not

↳ Exciting e^- into conduction band in semi-conductors:



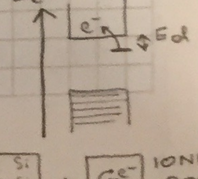
h^+ & e^- "Charge carriers"

i) Thermically: #$e^-_{FREE} = N_i \cdot \exp(-\frac{E_{GAP}}{k_B T})$

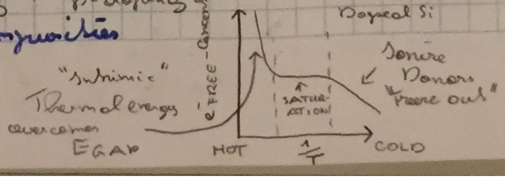
ii) Optically: $h\nu > E_{GAP}$

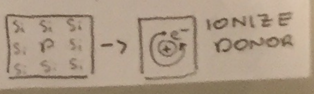
iii) Doping: #e^-_{FREE} / #h^+_{FREE} $= N_D \cdot \exp(-\frac{E_D}{k_B T})$

(n-doping / p-doping; Concentration of impurities; Ionization energy of dopant (= binding energy))



↳ Doping: Adding impurities



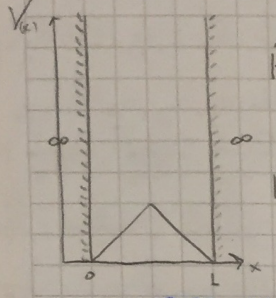


$\hat{H}$ is MATRIX? → DO NOT FORGET CONSTANT FACTOR IN EIGENVALUES !!!

⚠ → $\vec{v}\begin{pmatrix}\cdot\\\cdot\\\cdot\end{pmatrix}$

Time-Independent Perturbation Theory:

↳ NON-DEGENERATE: → Known Problem: $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$, $\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm}$



$\hat{H}^0 = \begin{cases} 0, & x\in[0,L] \\ \infty, & \text{else} \end{cases}$

$\hat{H}' = \begin{cases} x, & x\in[0,\frac{L}{2}] \\ (L-x), & x\in[\frac{L}{2},L] \end{cases}$

→ Want to solve: $\hat{H}\psi_n = E_n\psi_n \Rightarrow$ Write $\hat{H} = \hat{H}^0 + \lambda\hat{H}'$

→ Taylor Expand: $\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots$ (→ 1st-order correction term for n-th eigenfunction)

$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots$ (→ 1st-order correction term for n-th energy)

→ Plug in: $(\hat{H}^0+\lambda\hat{H}')(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\dots) = (E_n^0+\lambda E_n^1+\lambda^2E_n^2+\dots)(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\dots)$

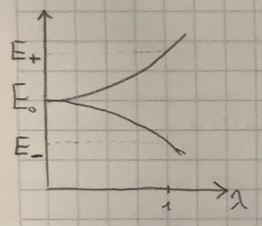
→ Collecting like-wise terms (Power Series are unique): λ: $\hat{H}^0\psi_n^1 + \hat{H}'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$

λ^2: $\hat{H}^0\psi_n^2 + \hat{H}'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0$

→ 1st-order: $\boxed{E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle}$, $\boxed{\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{(E_n^0-E_m^0)}\psi_m^0}$

→ 2nd-order: $\boxed{E_n^2 = \sum_{m\neq n}\frac{|\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle|^2}{(E_n^0-E_m^0)}}$

↳ DEGENERATE: → Starting Point: $\hat{H}^0\psi_a^0 = E^0\psi_a^0$, $\hat{H}^0\psi_b^0 = E^0\psi_b^0$, $\langle\psi_a^0|\psi_b^0\rangle = 0$



→ Note: $\psi_0 = \alpha\psi_a^0 + \beta\psi_b^0$ is still Eigenfunction with energy E^0

→ Same Procedure as above: $\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb}\end{pmatrix}\begin{pmatrix}\alpha\\\beta\end{pmatrix} = E^1\begin{pmatrix}\alpha\\\beta\end{pmatrix}$ → SIMPLE EIGENVALUES

$W_{ij} = \langle\psi_i^0|H'|\psi_j^0\rangle$

→ GENERAL RESULT: For n-degenerate: $\underline{\underline{W}} \in \mathbb{R}^{n\times n}$

The Variational Principle:

↳ For ANY trial function: $\langle H\rangle = \langle\psi_{TRIAL}|\hat{H}|\psi_{TRIAL}\rangle \geq E^{GROUND}_{STATE}$

↳ How to use: Choose NORMALIZED ψ_{TRIAL} with many adjustable parameters. Calculate $\langle H\rangle$ and use parameters to minimize → Upper bound for E_{GS}

↳ Proof: Assume real eigenfunctions to be complete & orthonormal: ψ_n

$\psi_{TRIAL} = \sum_n c_n\psi_n$ (since $\langle\psi_{TRIAL}|\psi_{TRIAL}\rangle = 1 \overset{(2)}{\overset{\Downarrow}{=}}{}^{(1)} \sum|c_n|^2$)

$\langle H\rangle = \langle\sum_n c_n\psi_n|\hat{H}\sum_m c_m\psi_m\rangle = \sum_n\sum_m c_n^* E_m c_m\langle\psi_n|\psi_m\rangle = \sum_m E_m|c_m|^2$

Per definition $E_{GS} \leq E_n\ \forall_n$ → $\langle H\rangle \geq E_{GS}$ $\left(\langle H\rangle = \sum_n|c_n|^2E_n = c_0^2E_0 + |c_1|^2E_1 + \dots \geq |c_0|^2E_0 + |c_1|^2E_0 + \dots = \sum|c_n|^2E_0 = E_0 \cdot 1\right)$

↳ Furthermore: If $\langle\psi_{TRIAL}|\psi^{GROUND}_{STATE}\rangle = 0 \Rightarrow \langle H\rangle \geq E_1$

↳ How to find a ψ_{TRIAL} orthogonal to ground state? If $V(x)$ is even in x, so will be ψ_{GS}, hence any odd ψ_{TRIAL} meets the condition

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VARIA:

↳ Gradients in different coord. sys.: $\vec{\nabla} = \begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}$, $\vec{\nabla}_{ZYL} = \begin{pmatrix}\frac{\partial}{\partial r}\\ \frac{1}{r}\frac{\partial}{\partial\varphi}\\ \frac{\partial}{\partial z}\end{pmatrix}$, $\vec{\nabla}_{SPH} = \begin{pmatrix}\frac{\partial}{\partial r}\\ \frac{1}{r}\frac{\partial}{\partial\vartheta}\\ \frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}\end{pmatrix}$

↳ Laplacian: $\vec{\nabla}^2 f = f_{xx} + f_{yy} + f_{zz}$

$\vec{\nabla}^2_{ZYL} f = \frac{1}{r}\frac{\partial}{\partial r}(r f_r) + \frac{1}{r^2}f_{\varphi\varphi} + f_{zz}$

$\vec{\nabla}^2_{SPH} f = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 f_r) + (r^2\sin\vartheta)^{-1}\frac{\partial}{\partial\vartheta}(\sin\vartheta\, f_\vartheta) + (r^2\sin^2\vartheta)^{-1}f_{\varphi\varphi}$

↳ 2 particle system: Change of var.: $\vec{r} = \vec{r}_1 - \vec{r}_2$, $\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2}$ … "center of mass"

Inverse Transform: $\vec{r}_1 = \vec{R} + \frac{\mu}{m_1}\vec{r}$, $\vec{r}_2 = \vec{R} - \frac{\mu}{m_2}\vec{r}$, $\mu = \frac{m_1m_2}{m_1+m_2}$ … "Reduced mass"

$\vec{\nabla}_1 = \left(\frac{\mu}{m_1}\right)\vec{\nabla}_R + \vec{\nabla}_r$, $\vec{\nabla}_2 = \left(\frac{\mu}{m_2}\right)\vec{\nabla}_R - \vec{\nabla}_r$

"Quanta": "Energy packages"
Parallelism: Single-electron configs.
Orthohelium: Triplet configs.