Quantum Physics 1
Class 27.

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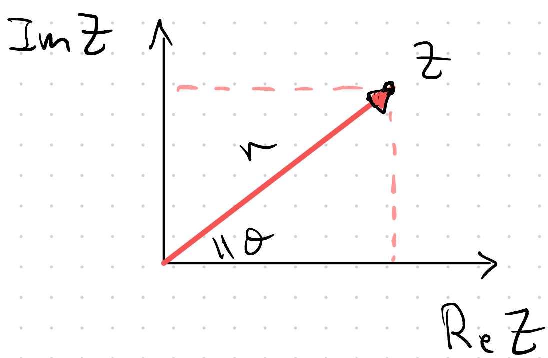
Quantum physics Review

The language of life at the nanoscale

Math Background

- Euler formula: $z = re^{i\theta}$, $i = \sqrt{-1}$



- Solving P.D.E.s
  1. Ansatz!
  2. Boundary conditions
  3. Separation of variables

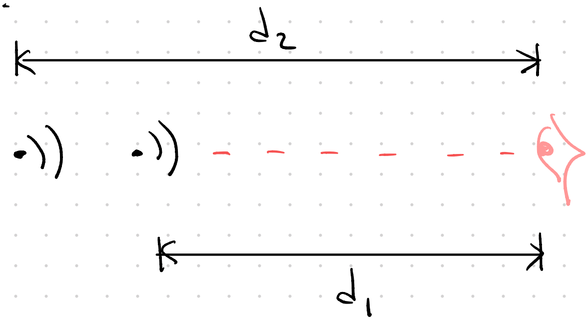
- Light is a wave:

$$\frac{\partial^2 E(x,t)}{\partial x^2} + \frac{-1}{c^2}\frac{\partial^2 E(x,t)}{\partial t^2} = 0$$

$$E(x,t) = Q(x)\,\phi(t)$$; guess:

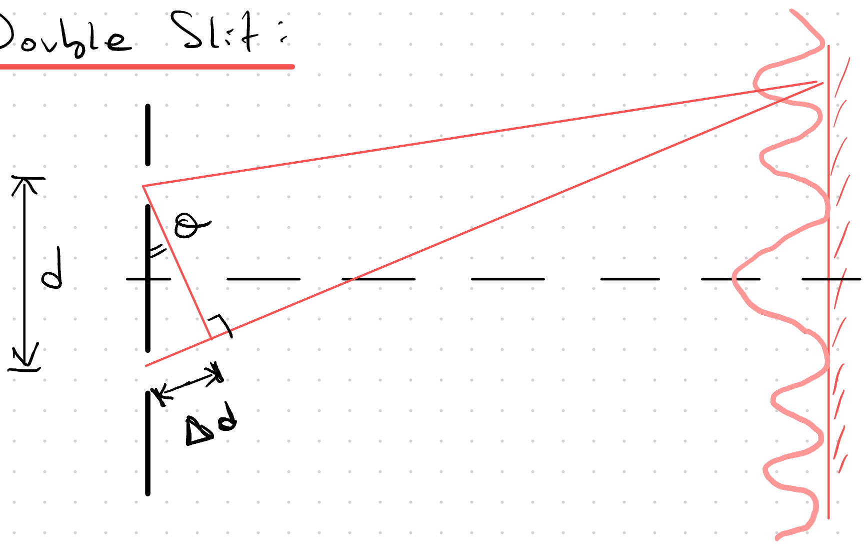
$$E(x,t) = e^{\pm i(kx - \omega t)}$$

Interference:



$$E(d,0) = e^{ikd_1}\left(1 + e^{ik\Delta d}\right)$$

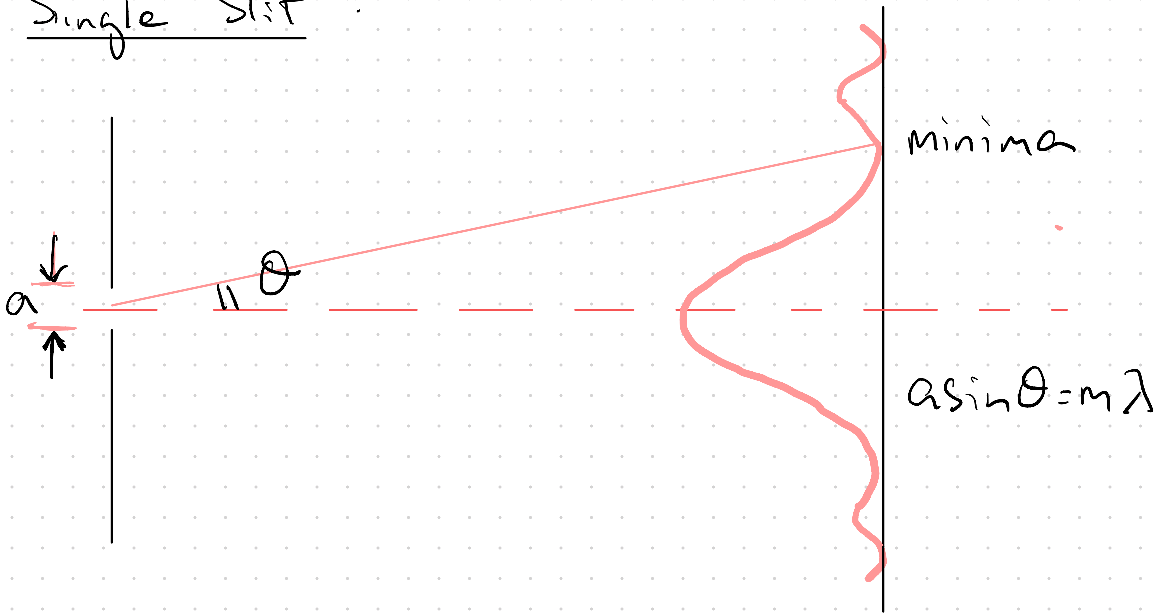
Double Slit:



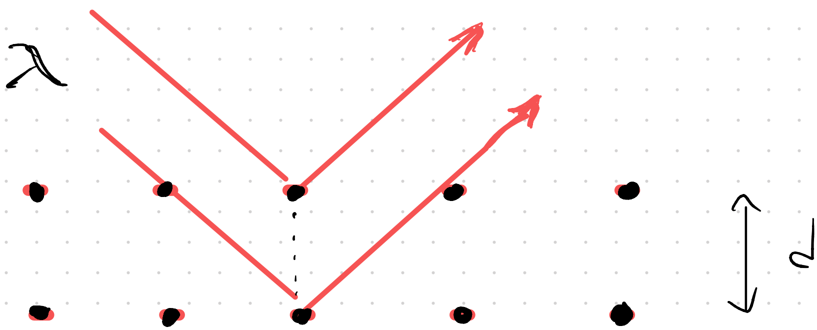
Constructive interference maxima

$$d\sin\theta = n\lambda$$

Single Slit :

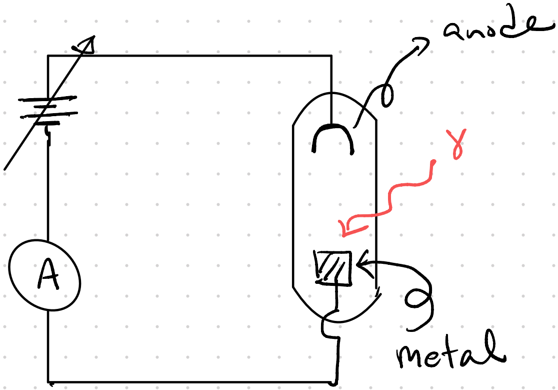


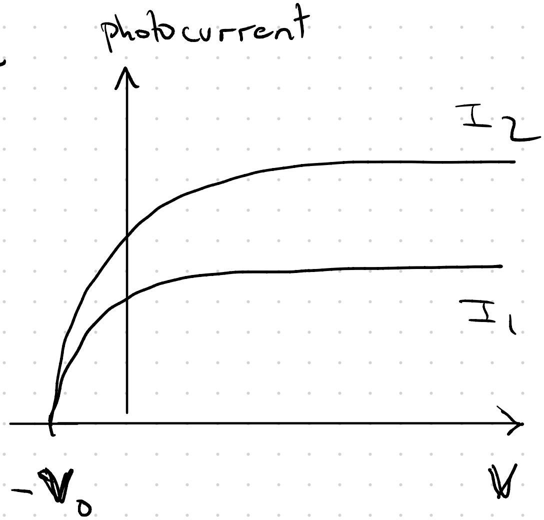
X-ray diffraction from crystals



$$\sin\theta = \frac{n\lambda}{2d} \; ; \quad d = \text{lattice constant}$$

Photoelectric effect and particle nature of light '





$$\boxed{h\nu = W + K}$$

W ≡ workfunction of the metal.

Wave nature of matter

- de Broglie λ : $\lambda = h/p$
- Interference of matter : e^-, p, etc.
- "Estimate" of uncertainty principle :

$$\boxed{\Delta y \, \Delta p \sim h}$$

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

$\Psi(x,t) \equiv$ probability amplitude of finding particle at x, t

$|\Psi(x,t)|^2 \sim$ probability density

$$\int |\Psi(x,t)|^2 \, dx = 1$$

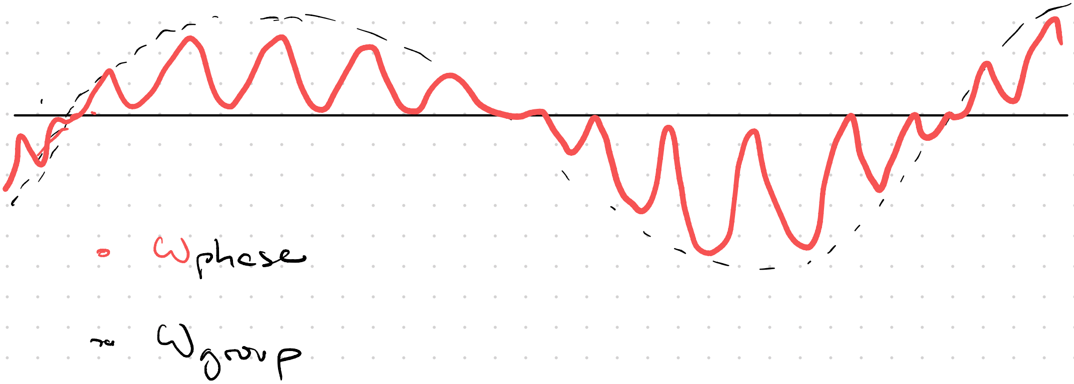
Now, $\Psi(x,t) \sim e^{i(kx-\omega t)}$

- Represents matter wave?
- Wave packets $\rightarrow$ superposition of waves.

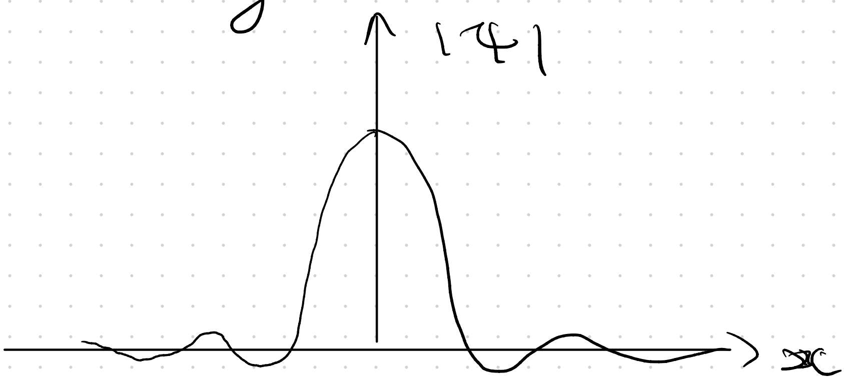
example:

$$\Psi_{tot} = \sin\left[\left(k - \frac{\Delta k}{2}\right)x - \left(\omega - \frac{\Delta \omega}{2}\right)t\right] + \sin\left[\left(k - \frac{\Delta k}{2}\right)x - \left(\omega - \frac{\Delta\omega}{2}\right)t\right]$$

$$= \sin(kx-\omega t)\cos\left[(\Delta k/2)x - (\Delta\omega/2)t\right]$$



6 Sum of many waves:



Quantum Mechanics "Basics"

$$\langle x \rangle = \sum_i prob_i \, x_i$$

$$= \int \Psi^* x \Psi \, dx$$

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx$$

$$\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2$$

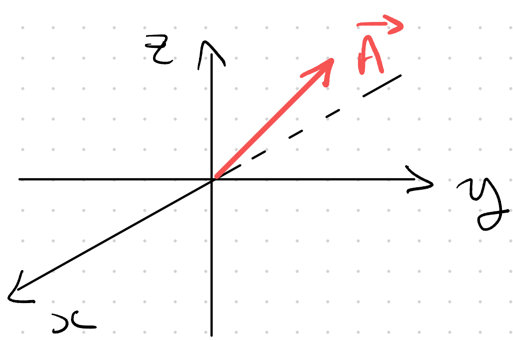
$$\Delta x \Delta p \geq \hbar/2$$

Time independent S.E. :

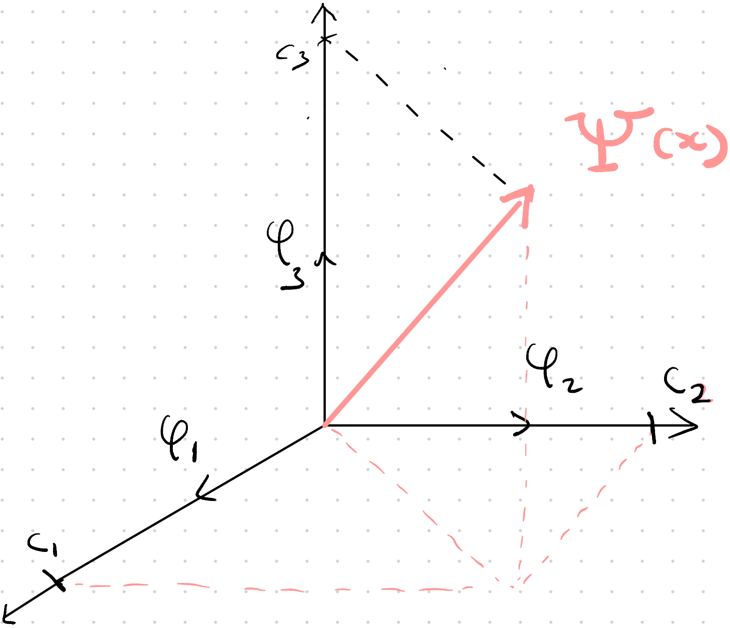
$$\left.\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) &= E\psi(x) \\ \frac{\partial f(t)}{\partial t} &= -\frac{iE}{\hbar} f(t) \end{aligned}\right\} \text{Separation of Variables}$$

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

Functional Vector Space



$$\vec{A} = A_x \hat{i} + A_y \hat{j} + A_z \hat{k}$$



$$\Psi(x) = \sum c_n \varphi_n$$

$$\int \varphi_m^* \varphi_n \, dx = 1$$

$$c_m = \int \varphi_m^* \Psi(x) \, dx$$

Energy Eigenvalue Problem:

$$\hat{H} \varphi(x) = E \varphi(x)$$

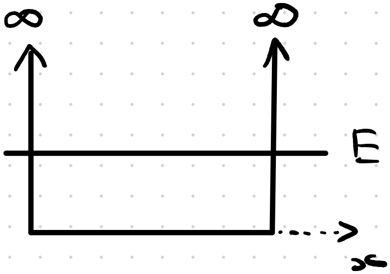
energy operator

eigenfunction

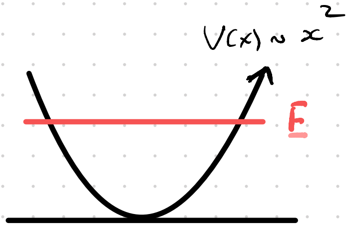
eigenvalue

In General: $\boxed{\hat{A} \varphi_a = a \varphi_a}$ eg) $\hat{A} : \hat{H}, \hat{p}, \hat{x}, \hat{L}, \ldots$

Bound State Problems :



Infinite Square Well



Harmonic oscillator

Finite Square Well.

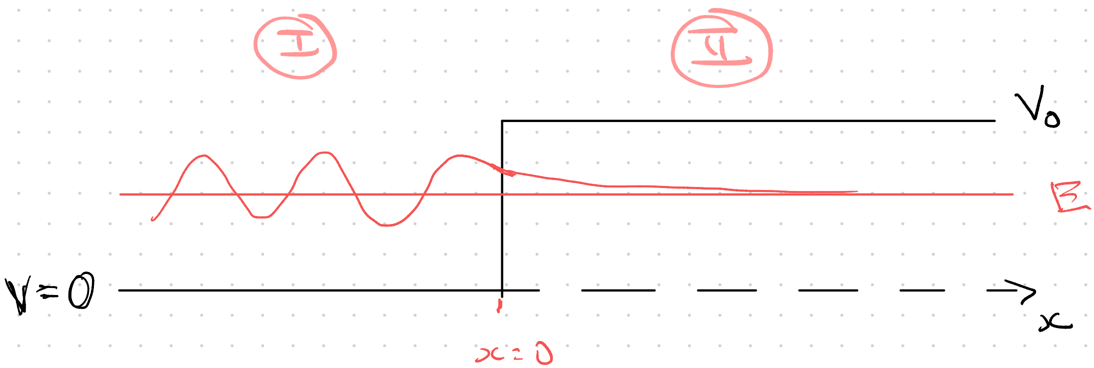
$$\left\{ \begin{array}{l} \varphi_n \sim \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \\ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \end{array} \right.$$

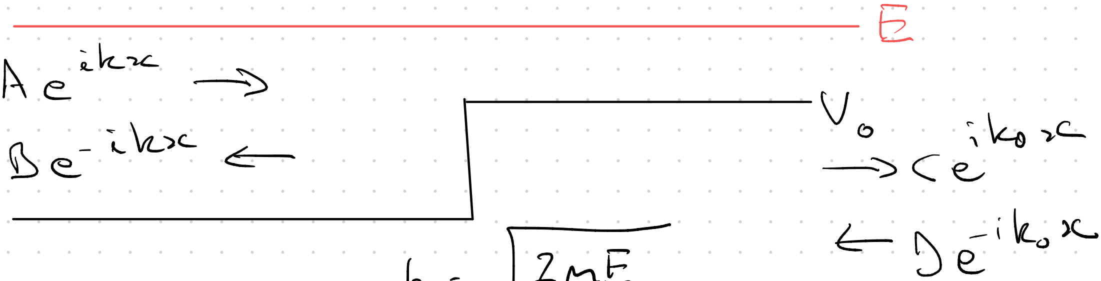
$$\left\{ \begin{array}{l} \varphi_n \sim H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} \\ E_n = (n+1/2)\hbar\omega \end{array} \right.$$

{ No Analytical Solution.

★ key element : boundary conditions

Scattering from Stepped Potential



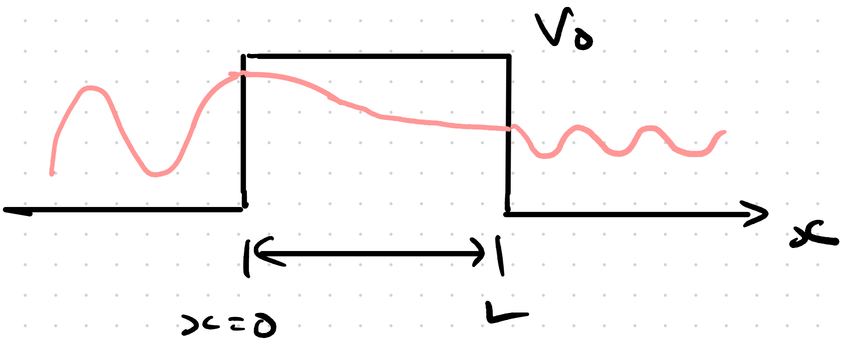


$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$k_0 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$R = \frac{j_{ref}}{j_{inc}}, \quad T = \frac{j_{trans}}{j_{inc}}$$

Quantum Tunneling



$$T = \frac{|C|^2}{|A|^2} = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\kappa L}; \quad \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

Principles of QM

- Hermitian operators
  - → operators linked to observables
  - → Eigenfunctions orthogonal
  - → " form complete set.

- $$\int \varphi^* (A\varphi)\, dx = \int (A\varphi)^* \psi \, dx$$

- Matrix representation

eg) $$\langle A \rangle = \int \psi^* \hat{A} \psi \, dx$$

$$= (c_1^* \; c_2^* \; \ldots) \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & \ddots & \\ \vdots & & \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

- Commutation relations

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

e.g) $$[\hat{x}, \hat{p}] = i\hbar$$

$$\frac{d\langle A \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle$$

3D Problems

Cartesian: 1D to 3D

· spherical coord.

Examples:

· 3D Box

· H-atom

etc.

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V(r))\psi$$

$$\left(\frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2}\right)\psi = (E-V)\psi$$

$$\psi(r,\theta,\phi) = \underbrace{R(r)}_{\text{radial basis funct.}}\underbrace{Y(\theta,\phi)}_{\Theta(\theta)\Phi(\phi)}$$

spherical harmonics

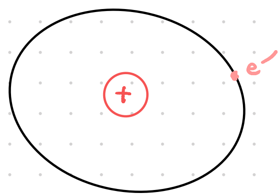
radial basis funct.

Legendre polynomials

Angular Momentum

- $\vec{L} = \vec{r} \times \vec{p}$
- $\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \longrightarrow \hat{L}_z \Phi = m\hbar \Phi$
- $\hat{L}^2 Y(\theta, \phi) = l(l+1) \hbar^2 Y(\theta, \phi)$
- $[\hat{L}^2, \hat{L}_z] = 0$
- $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$

Hydrogen Atom

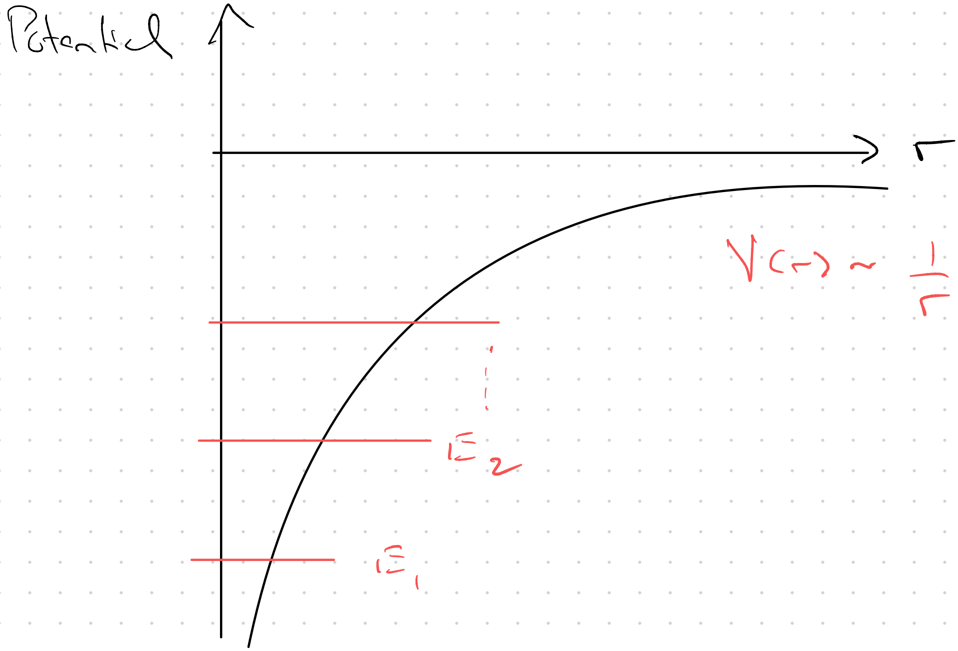


$$\Psi(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi)$$

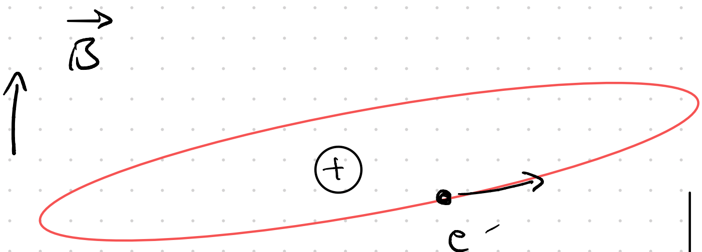
$$V(r) = \frac{-Ze^2}{4\pi \varepsilon_0 r} ; \quad Z = 1$$

$$R(r) = r^l F_n(r) e^{-\sqrt{2m_0 E/\hbar^2}\, r}$$

$$E_n = \frac{-(13.6\,eV) Z^2}{n^2} ; \quad n = 1, 2, 3, \ldots$$



Zeeman Effect

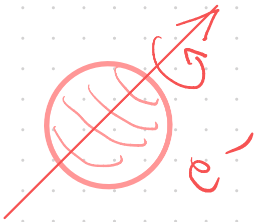


$$U = -\vec{\mu} \cdot \vec{B}$$

$$\hat{H} = -\vec{\mu} \cdot \vec{B}$$

$$\boxed{\vec{\mu} = \frac{q}{2m_0} \hat{L}}$$

Intrinsic Spin



$\vec{\mu} = g \frac{\mu_B}{\hbar} \vec{S}$; Stern-Gerlach experiment

$|\vec{S}| = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\,\hbar$

$s = 1/2$; $g \equiv$ g-factor

$\psi(x,t) \longrightarrow \psi(x,t)\,\chi(t)$

$$\boxed{\hat{H} = -\vec{\mu}_s \cdot \vec{B}}$$

- Qubits (Bloch sphere)
- Relativity + QM
- NMR