Closing: What have we done and What's next?

- Motivated wave nature of particle via two-slit experiment
- Ψ the wavefunction and how to use it through analogy of light
- Physical interpretation involves $|\Psi|^2$
- Time-dependent Schrödinger Equation governs time evolution
- Time-independent Schrödinger Equation is eigenvalue problem of the Hamiltonian operator $\hat{H}$
- To construct $\hat{H}$, think classical (what is Hamiltonian classically) and go quantum by substituting $\hat{x} \to x$ and $\hat{p} \to \frac{\hbar}{i}\frac{d}{dx}$

- Other operators are constructed similarly
- Dirac: QM is $[\hat{x}, \hat{p}] = i\hbar$, regardless how it is realized
- Standard TISE problems
  - 1D infinite well (particle-in-a-box)
    finite well
    harmonic oscillator
    "2D" rigid rotor (ϕ only)

  Math technique: imposing boundary conditions to connect solutions in different regions
  Series solution
  Well-behaved wavefunction

- 2D/3D Infinite wells

Spherically symmetric $U(r)$

[Math technique: Separation of Variables]

θ, ϕ angular part: $\underbrace{Y_{\ell m_\ell}(\theta,\phi)}_{\sim P_\ell^{|m_\ell|}(\cos\theta)\cdot e^{i m_\ell \phi}}$ Spherical Harmonics

$R_{n\ell}(r)$ depends on $U(r)$

$\underbrace{m_\ell = \ell, \ell-1, \cdots, 0, \cdots, -\ell}_{\text{degeneracy}}$

$$\psi_{n\ell m_\ell}(r,\theta,\phi) = R_{n\ell}(r)\, Y_{\ell m_\ell}(\theta,\phi)$$

- Hydrogen atom $\quad U(r) = -\dfrac{e^2}{4\pi\varepsilon_0 r}$

$$E_{n\ell} = E_n = -\frac{13.6}{n^2}\text{ eV}$$ with "13.6" coming from a combination of constants

higher degeneracy than usual $U(r)$

- Orbital Angular Momentum
  - $\hat{L}_x, \hat{L}_y, \hat{L}_z, \hat{L}^2$ commutation relations
  - $[\hat{L}^2, \hat{L}_z] = 0 \Rightarrow$ share common eigenstates
  - $$\left.\begin{aligned} \hat{L}^2 Y_{\ell m_\ell} &= \ell(\ell+1)\hbar^2\, Y_{\ell m_\ell} \\ \hat{L}_z Y_{\ell m_\ell} &= m_\ell\hbar\, Y_{\ell m_\ell} \end{aligned}\right\}$$ Unusual properties of orbital AM and Vector Model

- General Angular Momentum in QM
  - defined by $\hat{J}_x, \hat{J}_y, \hat{J}_z, \hat{J}^2$ commutation relations
  - $[\hat{J}^2, \hat{J}_z] = 0 \Rightarrow$ share common eigenstates
  - $\hat{J}^2 |j, m_j\rangle = j(j+1)\hbar^2 |j, m_j\rangle$

    with j being either integers OR half-integers
  - $\hat{J}_z |j, m_j\rangle = m_j \hbar |j, m_j\rangle$

    with $m_j = \underbrace{j, j-1, \cdots, -j+1, -j}_{(2j+1) \text{ values}}$ for given j
  - Orbital AM is a special case with j taking on integers only

- Operators
  - Physical quantity is represented by operator
  - Hermitian Operators
  - Eigenvalues of Hermitian operator are real and eigenstates can be made orthogonal
  - Expansion of a general state in a complete set of states
  - Ordering of operators is important
  - $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
  - General Uncertainty Relation

- Measurement Theory
  - Measure A, outcome is an eigenvalue of $\hat{A}$ and state collapses to corresponding eigenstate
  - If state on which measurement is made is known,

$$\Psi = \sum_i c_i \varphi_i \qquad \hat{A}\varphi_i = a_i \varphi_i$$

$|c_i|^2$ = Prob. of getting a_i

$\langle \hat{A} \rangle$ = Expectation Value $= \int \Psi^* \hat{A} \Psi \, d\tau = \langle \Psi | \hat{A} | \Psi \rangle$

$$(\Delta A)^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

(ΔA) is the uncertainty that goes into the uncertainty relation

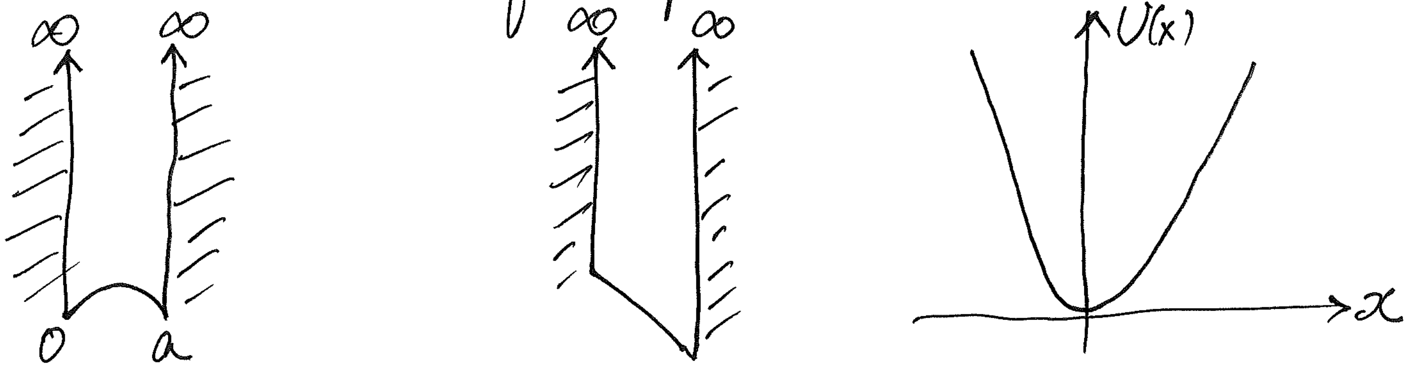
Behind expectation value is the idea of measurements on identical copies

- Spin angular momentum of electron
  - Stern-Gerlach experiment
  - intrinsic property → $\sqrt{\frac{3}{4}}\hbar$ in magnitude
    → $+\frac{\hbar}{2}$, $-\frac{\hbar}{2}$ for component
  - 2×2 matrices for $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}^2$ & Pauli matrices
  - Eigenvalues and eigenstates of $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$
  - Playground of QM
  - Illustrates QM
  - Spin (Larmor) Precession in Magnetic Field
- Postulates of Quantum Mechanics

- TISE and eigenvalue problems can be formulated into matrix problems

What's Next?

- How about TISE for problems that can't be solved analytically?



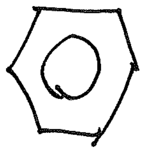
- How about many-electron systems?

  He atom? Li atom? . . .

- How about molecules?

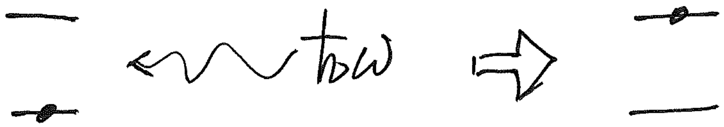
  Chemical bond

  H_2



What is it?

- Why are there transitions?



$$\hat{H}_{atom} + \underbrace{\text{EM term}}_{\sim \mathcal{E}_0 x \cos\omega t} \qquad \text{time-dependent term}$$

<u>Need</u>

- Approximation Methods
    - Variation Method
    - Time-independent Perturbation Theory
    - Time-dependent Perturbation Theory

This is the <u>next course</u> — <u>Applied Quantum Mechanics</u>