Purpose of the course
+ quantum mechanics is a paradigm shift
  a fundamentally new look at nature

+ P3316 is about key ideas of QM
  - quantized energy levels
  - particle/wave duality for light & matter
  - plus essential math formalism that incorporates
    these ideas into "wave mechanics"

+ P3317 surveys what consequences the new
  vision of nature has for physical phenomena:
  - atoms, molecules, solids, radiation, nuclei,
    elem. part.

+ You get wide exposure to real-life physics
  - only enough time to survey many topics
  - facts/jargon: necessary to talk to other physicists

+ Computer project/exercises: (MATLAB, ptylab)
  indispensable skill for any physicist/engineer

+ Seminars:
  - presentation skills
  - reading of scientific papers
  - lots of exciting physics

Review of Wave Mechanics Formalism

1. Linear algebra on function spaces
   + "vector" $|\psi\rangle = \text{function } \psi(x)$

\[ \psi(x) = \langle x | \psi \rangle \]

Formally:

\[ \psi(x) = \langle x | \psi \rangle \]

\[ |\psi\rangle = \begin{pmatrix} \psi(x_1) \delta x \\ \psi(x_2) \delta x \\ \vdots \end{pmatrix} \]

Ket = column

Hilbert space

States & operators

position space

momentum space

spin space
inner product $\langle \psi_1 | \psi_2 \rangle = \int \psi_1^*(r) \psi_2(r) \, dr$

$|\psi\rangle^\dagger = \langle \psi |$ adjoint, \[ \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = (c_1^* c_2^* c_3^* \ldots) \]

norm: $\langle \psi | \psi \rangle = \int \psi^*(r) \psi(r) \, dr = \int |\psi(r)|^2 \, dr$

operator $\hat{A} |\psi_1\rangle = |\psi_2\rangle$

linear: $\hat{A} (\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle) = \lambda_1 \hat{A} |\psi_1\rangle + \lambda_2 \hat{A} |\psi_2\rangle$

Hermitian: $\langle \hat{A} |\psi_1 |\psi_2 \rangle = \langle \psi_1 |\hat{A} |\psi_2 \rangle = \langle \psi_1 |\hat{A}^\dagger |\psi_2 \rangle$

(2) QM observables

Classically $\mathbf{F}, \mathbf{p}$ - state

$A(\mathbf{r}, \mathbf{p})$ - observable (e.g. energy, ang. momentum)

Eigenstates $\{\phi_n\}$: $\hat{A} |\phi_n\rangle = A_n |\phi_n\rangle$

$\{A_n\}$ - spectrum of $\hat{A}$ (finite or infinite length)

$\{ |\phi_n\rangle \}$ - form complete orthonormal basis

$\langle \phi_n | \phi_m \rangle = \delta_{nm}$ - Kronecker delta

(3) Measurement of $\hat{A}$ for a state $|\psi\rangle$

possible outcome is spectrum of $\hat{A}$

$p(A = A_n) = |\langle \phi_n | \psi \rangle|^2$

after measurement: $|\psi\rangle \rightarrow |\phi_n\rangle$

"collapse"

expectation values:

$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$

$\langle \hat{A}^2 \rangle = \langle \psi | \hat{A}^2 | \psi \rangle$

etc.
4. Matrix representation of $\hat{A}$

\[
\hat{A}|f> = |g>
\]

\[
|g> = \sum_i \langle \psi_i | g> | \psi_i >
\]

\[
d_i = \sum_j A_{ij} c_j
\]

\[
|f> = \sum_j \langle \psi_j | f> | \psi_j >
\]

\[
A_{ij} = \langle \psi_i | \hat{A} | \psi_j >
\]

5. Important Square Matrices

Hermitian (self-adjoint) $A^+=A$ ($A_{ij} = A_{ji}^*$)

* Real spectrum (eigenvalues)
* Complete & orthogonal set of eigenvectors

All operators of observables

Unitary $A^{-1} = A^+$

* Eigenvalues have unit magnitude (but complex)
* Eigenvectors orthogonal
* Preserves lengths & angles of vectors

E.g. time evolution operator (next lecture)
or to "change basis"

6. Fancier matrices: creation, annihilation operators

Neither Hermitian nor unitary (but have other symmetries) more later

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Example: numerical soln. of 1D Schrödinger eqn.

\[\hat{H}\psi_n = E_n \psi_n, \quad \text{with} \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(x)\]

\[\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{x} = x\]

$V(x=0) \to \infty$

$V(x=L) \to \infty$

$\psi(x)$: represented on a grid $x_j = j\hbar_\omega$, $j=0,1,...,N$ ($N\hbar_\omega = L$)

$V(x): \quad n \quad n \quad n$

Differential operator:

\[
\frac{d}{dx} \psi(x_j) \approx \frac{\psi(x_{j+1}) - \psi(x_{j-1})}{2\hbar_\omega}
\]
\[
\begin{align*}
\text{e.g. matrix form} \quad P_x &= \frac{\hbar}{2}\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots \\
-1 & 0 & 1 & 0 & \cdots \\
0 & -1 & 0 & 1 & \cdots \\
0 & 0 & -1 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
\end{align*}
\]

Can write matrix for \( H \) HW prob

use numerical matrix packages to find eigenvalues \((E_n)\) and eigenvectors \(\psi_n(x_j)\)