Purpose of the course

* quantum mechanics is a <u>paradigm shift</u>
  a fundamentally new look at nature

* P3316 is about <u>key ideas</u> of Q.M.
  - quantized energy levels
  - particle/wave duality for light & matter
  - plus essential math formalism that incorporates these ideas into "wave mechanics"

* P3317 surveys what <u>consequences</u> 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 <u>survey</u> many topics :(:)
  - facts / jargon : necessary to talk to other physicists

* Computer project / exercises : (MATLAB, pylab)
  indispensable skill for any physicist / engineer

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

Review of Wave Mechanics Formalism

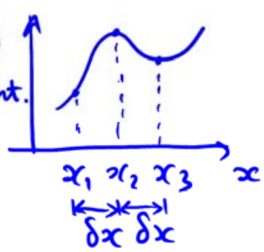
states & operators

① Linear algebra on function spaces

* <u>"vector"</u> $|\psi\rangle$ = function $\underbrace{\psi(\vec{r})}_{\text{Hilbert space}}$

position space
momentum space
spin space
....

e.g. $\psi(x)$
space represent.



$$\boxed{\text{Formally: } \psi(x) = \langle x|\psi\rangle}$$

$$|\psi\rangle = \begin{pmatrix} \psi(x_1)\sqrt{\delta x} \\ \psi(x_2)\sqrt{\delta x} \\ \psi(x_3)\sqrt{\delta x} \\ \vdots \end{pmatrix}$$

ket = column

inner product $\langle\psi_1|\psi_2\rangle = \int \psi_1^*(\vec{r})\psi_2(\vec{r})\,d\vec{r}$

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

bra
= row

norm: $\langle\psi|\psi\rangle = \int \psi^*(\vec{r})\psi(\vec{r})\,d\vec{r} = \int |\psi(\vec{r})|^2 d\vec{r}$
finite

* 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: $\langle\hat{A}\psi_1|\psi_2\rangle = \langle\psi_1|\hat{A}\psi_2\rangle \equiv \langle\psi_1|\hat{A}|\psi_2\rangle$

② QM observables

Classically

$\vec{r}, \vec{p}$ - state

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

Q.M.

$\psi(\vec{r})$ - state $\langle\psi|\psi\rangle = 1$

$\hat{A} = A(\hat{\vec{r}}, \hat{\vec{p}})$ - Hermitian operator ↔ real

* Eigenstates $|\psi_n\rangle$, eigenvalues a_n : $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$

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

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

$\langle\psi_n|\psi_m\rangle = \delta_{nm}$ ← Kronecker delta

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

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

$p(A = a_n) = |\langle\psi_n|\psi\rangle|^2$

* after measurement: $|\psi\rangle \to |\psi_n\rangle$
"collapse"

* expectation values: $\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle$

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

etc.

④ Matrix representation of $\hat{A}$

$\hat{A}|f\rangle = |g\rangle$; $|g\rangle = \sum_i \overbrace{\langle\psi_i|g\rangle}^{d_i}|\psi_i\rangle$

$|f\rangle = \sum_j \underbrace{\langle\psi_j|f\rangle}_{c_j}|\psi_j\rangle$

$d_i = \sum_j A_{ij} c_j$

$A_{ij} = \langle\psi_i|\hat{A}|\psi_j\rangle$

⑤ Important square matrices

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

* real spectrum (eigenvalues) ;
* complete & orthogonal set of eigenvectors

All operators of observables

Unitary $A^{-1} = A^\dagger$

* 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

Example : numerical soln. of 1D Schrödinger eqn.

$\hat{\mathcal{H}}\psi_n = E_n\psi_n$, with $\hat{\mathcal{H}} = \frac{\hat{p}_x^2}{2m} + V(\hat{x})$

$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$, $\hat{x} = x$. $V(x=0) \to \infty$

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

$\psi(x)$: represented on a grid $x_j = jh_0$, $j = 0, \dots, N$ $(Nh_0 = L)$

$V(x)$: — " — " — " —

differential operator : $\frac{d}{dx}\psi(x_j) \approx \frac{\psi(x_{j+1}) - \psi(x_{j-1})}{2h_0}$

e.g. in matrix form

$$p_x = \frac{\hbar}{2 i h_0} \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ -1 & 0 & 1 & 0 & \cdots \\ 0 & -1 & 0 & 1 & \cdots \\ 0 & 0 & -1 & 0 & \\ & \vdots & \vdots & \vdots & \end{pmatrix}$$

Can write matrix for $\hat{H}$ HW prob

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