Physics 522: Graduate Quantum Mechanics II

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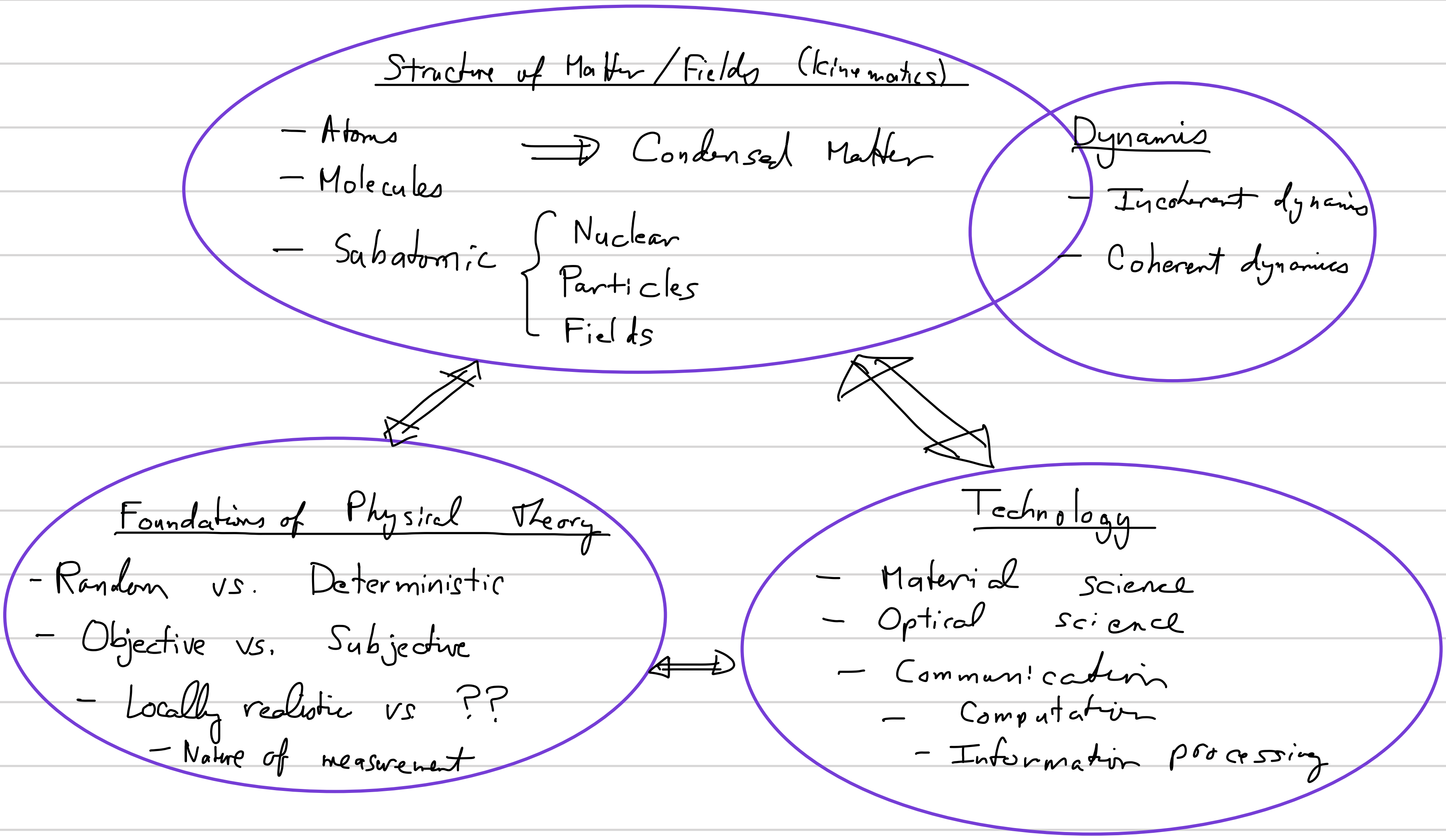
Lecture 1: Review of the Structure of Quantum Mechanics



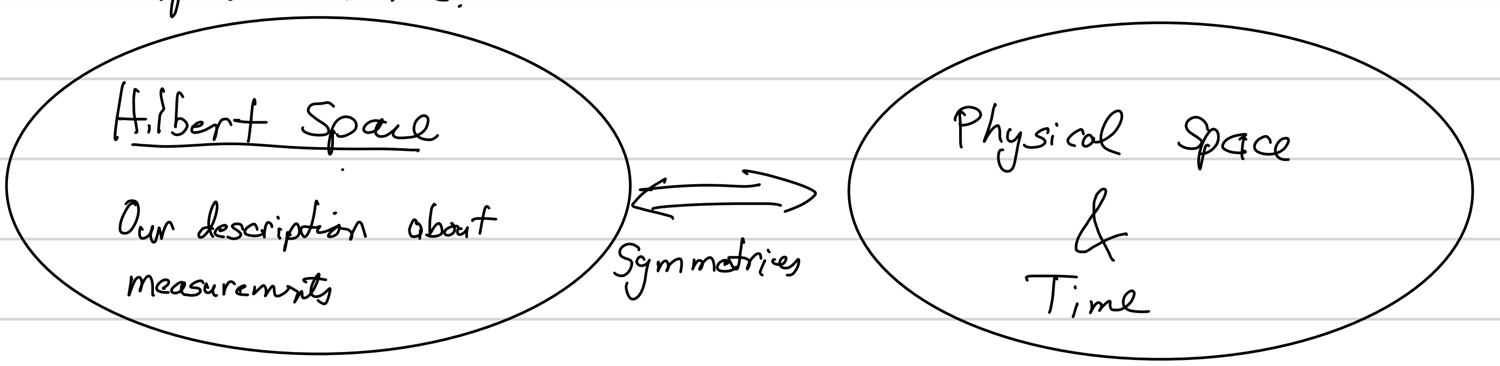
This was our "org chart" from 521. Last semester the focus was on the "Foundation of the Physical Theory." This semester of focus will be on the "Structure of matter." Our main focus will be on "ordinary matter"; atoms and molecules, with particular emphasis on atoms.

As we have seen, symmetries play a central role in connecting the physical degrees of freedom to Hilbert space and quantum observables. We will elaborate on the theory of symmetries and groups in much more detail, later in the semester. Symmetries will be a unifying concept throughout the semester. Of particular importance is the rotation group, which is intimately tied to the theory of vectors and tensor. The theory of angular momentum, the generator of rotations, will play a central role in this discussion.

Review: Basic Structure of Quantum Mechanics

Physical theory allows us to make predictions about the outcomes of experiments. In quantum theory, these predicts are only about the probabilities of seeing a given measurement outcome. That is, generally the measurement result is random. Unlike it classical statistical physics, where randomness arises for incomplete information, in quantum physics we believe this randomness is intrinsic. That is, even when we have maximum possible information, we still cannot necessarily predict the measurement outcome. This is quantum mechanics' greatest mystery.

Quantum mechanics thus has a mathematical structure with two essential parts: (i) An encoding of our predictions about the physical work; (ii) The connection to physical quantities. Ultimately, the latter teaches us about the structure of matter / fields and the building blocks of the universe.



Hilbert Space

- $\mathcal{H}$: Complex vector space, with an inner product, possibly infinite dimensional

  Vectors (kets) $\{|\psi\rangle\} \in \mathcal{H}$ (bras) $\{\langle\psi|\} \in \mathcal{H}_{dual}$

  Inner (dot) product $\langle\psi|\phi\rangle \in \mathbb{C}$ complex #

  Superposition $|\chi\rangle = a|\psi\rangle + b|\phi\rangle \in \mathcal{H}$

  $$\langle\chi| = a^*\langle\psi| + b^*\langle\phi| \in \mathcal{H}_{dual}$$

Basis: $\{|e_i\rangle \mid i=1,2,3\cdots d\}$: Linearly independent set that spans $\mathcal{H}$: $|\psi\rangle = \sum_{i=1}^{d} c_i |e_i\rangle$

Orthonormal basis: $\langle e_i|e_j\rangle = \delta_{ij} = (0 \; i\neq j, \; 1 \; i=j)$

$$\Rightarrow c_i = \langle e_i|\psi\rangle \Rightarrow |\psi\rangle = \sum_i \langle e_i|\psi\rangle |e_i\rangle = \sum_i |e_i\rangle\langle e_i|\psi\rangle \Rightarrow \sum_i |e_i\rangle\langle e_i| = \hat{\mathbb{1}}$$

Resolution of the identity

Linear operators on Hilbert space: $\hat{A}\,|\psi\rangle = |\phi\rangle \in \mathcal{H}$

$$\hat{A}\left(a|\psi\rangle + b|\phi\rangle\right) = a\,\hat{A}|\psi\rangle + b\,\hat{A}|\phi\rangle$$

Eigenvectors / eigenvalues: $\hat{A}|a\rangle = a|a\rangle$

Adjoint: if $\hat{A}|\psi\rangle = |\phi\rangle$, then $\langle\psi|\hat{A}^{\dagger} = \langle\phi|$

Hermitian operator: $\hat{A} = \hat{A}^{\dagger} \Rightarrow$ eigenvalues real, eigenvectors can form orthonormal basis

Unitary operator $\hat{U}$: $\hat{U}^{\dagger}\hat{U} = \hat{U}\hat{U}^{\dagger} = \hat{\mathbb{1}}$

$\Rightarrow$ If $|\psi'\rangle = \hat{U}|\psi\rangle$, $|\phi'\rangle = \hat{U}|\phi\rangle$ $\langle\psi'|\phi'\rangle = \langle\psi|\hat{U}^{\dagger}\hat{U}|\phi\rangle = \langle\psi|\phi\rangle$

$\Rightarrow$ Unitary operators preserve inner product.

Unitary operator "generated" by a Hermitian Operator: $\hat{U}(\lambda) = e^{i\lambda\hat{A}}$ Real #

$$\hat{U}(\lambda) = \hat{\mathbb{1}} + i\lambda\hat{A} + \frac{1}{2}(i\lambda)^2\hat{A}^2 + \cdots \frac{1}{n!}(i\lambda)^n\hat{A}^n + \cdots$$

Representations in a basis $\{|e_\alpha\rangle \mid \alpha = 1, 2, \cdots d\}$

$c_\alpha \equiv \langle e_\alpha|\psi\rangle \Rightarrow |\psi\rangle \doteq \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{bmatrix}$ Column vector

$c_\alpha^* = \langle\psi|e_\alpha\rangle \Rightarrow \langle\psi| \doteq [c_1^*, c_2^*, \cdots, c_d^*]$ row vector

Matrix elements: $A_{\alpha\alpha'} \equiv \langle e_\alpha|\hat{A}|e_{\alpha'}\rangle \Rightarrow \hat{A} \doteq \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1d} \\ A_{21} & A_{22} & \cdots & A_{2d} \\ \vdots & & & \\ A_{d1} & \cdots & \cdots & A_{dd} \end{bmatrix}$

$$(A^{\dagger})_{\alpha\alpha'} = A^*_{\alpha\alpha'} = (A^{T*})_{\alpha\alpha'}$$

Change of basis $\{|f_\beta\rangle \mid \beta = 1, 2, \cdots d\}$

New representation: $\tilde{c}_\beta \equiv \langle f_\beta|\psi\rangle$; $\tilde{A}_{\beta\beta'} \equiv \langle f_\beta|\hat{A}|f_{\beta'}\rangle$

Relate different representations by inserting a resolution of the identity:

$$\tilde{c}_\beta = \langle f_\beta|\hat{\mathbb{1}}|\psi\rangle = \sum_\alpha \underbrace{\langle f_\beta|e_\alpha\rangle}_{S_{\beta\alpha}:\ \text{Unitary}}\langle e_\alpha|\psi\rangle = \sum S_{\beta\alpha}\, c_\alpha \quad : \text{Similarity transform}$$

$$\tilde{A}_{\beta\beta'} = \langle f_\beta|\hat{\mathbb{1}}\hat{A}\hat{\mathbb{1}}|f_{\beta'}\rangle = \sum_{\alpha,\alpha'}\langle f_\beta|e_\alpha\rangle\langle e_\alpha|\hat{A}|e_{\alpha'}\rangle\langle e_{\alpha'}|f_{\beta'}\rangle = \sum_{\alpha,\alpha'}(S_{\beta\alpha})\,A_{\alpha\alpha'}\,(S_{\beta\alpha'})^{\dagger}$$

• **States**: Our "state of knowledge" about the system (like a probability distribution).

- Pure state: Maximal knowledge about a quantum system $\Leftrightarrow$ Vector in Hilbert space

$$|\psi\rangle \in \mathcal{H}$$

Really equivalence class - ray in Hilbert space: Normalize $\||\psi\|| = \sqrt{\langle\psi|\psi\rangle} = 1$

Normalization still leaves overall phase undefined: $|\psi\rangle \equiv e^{i\phi}|\psi\rangle$

Born rule (simple statement). Given we describe the state by $|\psi\rangle$, the probability of finding the system in state $|\alpha\rangle$ after a "measurement is"

$$P(\alpha|\psi) = |\underbrace{\langle\alpha|\psi\rangle}_{\text{"Probabity amplitude"}}|^2$$

Note if $|\psi\rangle = a|\phi_1\rangle + b|\phi_2\rangle$, $\langle\phi_1|\phi_2\rangle = 0 \Rightarrow P(\alpha|\psi) = |a\langle\alpha|\phi_1\rangle + b\langle\alpha|\phi_2\rangle|^2$

$$= \underbrace{|a|^2}_{P(\phi_1)} \underbrace{|\langle\alpha|\phi_1\rangle|^2}_{P(\alpha|\phi_1)} + \underbrace{|b|^2}_{P(\phi_2)} \underbrace{|\langle\alpha|\phi_2\rangle|^2}_{P(\alpha|\phi_2)} + \underbrace{ab^* \langle\alpha|\phi_1\rangle\langle\phi_2|\beta\rangle + a^*b\langle\alpha|\phi_2\rangle\langle\phi_1|\alpha\rangle}_{\text{Quantum Interference}}$$

- Mixed states: Incomplete knowledge about a quantum system

Note: For a pure state, $P(\alpha|\psi) = \langle\alpha|\psi\rangle\langle\psi|\alpha\rangle \equiv \langle\alpha|\hat{\rho}|\alpha\rangle$

$\Rightarrow$ State is the "density operator" $\hat{\rho} = |\psi\rangle\langle\psi|$

Mixed State: Statistical mixture of pure states: $\{\underbrace{P_\psi}_{\text{"classical" probability}}, |\psi\rangle\}$

$$\Rightarrow P(\alpha) = \sum_\psi P_\psi P(\alpha|\psi) = \sum_\alpha P_\psi \langle\alpha|\psi\rangle\langle\psi|\alpha\rangle = \langle\alpha|\left(\sum_\psi P_\psi |\psi\rangle\langle\psi|\right)|\alpha\rangle$$

$\Rightarrow$ General state: Density operator $\hat{\rho} = \sum_\psi P_\psi |\psi\rangle\langle\psi|$

$$P(\alpha) = \langle\alpha|\hat{\rho}|\alpha\rangle$$

Measurement:

- Born rule

Any measurement has a series of possible outcomes $\{\alpha\}$. Each measurement outcome occurs with a probability $p(\alpha)$. We require $\sum_\alpha p(\alpha) = 1$.
To each possible measure outcome we assign an operator $\hat{E}_\alpha$ such that $\sum_\alpha' \hat{E}_\alpha = \hat{\mathbb{1}}$ (resolution of the identity).

The basic measurements in quantum mechanics correspond to a measurement in an "orthornomal basis" $\{|e_\alpha\rangle\}$

$$\Rightarrow \hat{E}_\alpha = |e_\alpha\rangle\langle e_\alpha|, \qquad \sum_\alpha \hat{E}_\alpha = \hat{\mathbb{1}} \quad : \text{technically this is a "POVM"}$$

$$p(\alpha) = \langle\alpha|\hat{\rho}|\alpha\rangle = \underset{\text{trace}}{\mathrm{Tr}}(\hat{\rho}\;|\alpha\rangle\langle\alpha|) = \mathrm{tr}(\hat{\rho}\,\hat{E}_\alpha) \quad \underline{\text{General Born rule}}$$

Measurement in orthonormal basis is often called measurement of a Hermitian operator because we can associate the orthonormal basis with its eigenvectors.

$$\text{Let} \quad \hat{A} = \sum \alpha\, |e_\alpha\rangle\langle e_\alpha|$$

$\Rightarrow$ One often says one measures the "observable" $\hat{A}$, which is a Hermitian operator. Each outcome is labeled by an eigenvalue of $\hat{A}$, α, which is a real number. The probability of "finding α" is $|\langle\alpha|\psi\rangle|^2$ for a pure state and $\langle\alpha|\hat{\rho}|\alpha\rangle$ more generally.

- Compatible and Incompatible observables

Two observables $\hat{A}$ & $\hat{B}$ that have the same eigenvectors are said to be "compatible". That is we can measure in a basis, and learn about the eigenvalues of either. Compatible observables <u>commute</u>: $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$

The expected value of a measurement: $\langle\hat{A}\rangle = \sum \alpha\, p(\alpha) = \langle\psi|\hat{A}|\psi\rangle$

The uncertainty variance $\Delta A^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$

The uncertainty relation: $\Delta A\, \Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$