IV. Foundations of Quantum Mechanics

IV.1 Axioms Revisited

* We note that the wave mechanics developed in chapter I satisfies the axioms (Q1–Q4) first proposed in I.1. In particular, wave functions ψ = vectors in a concrete Hilbert space (like $L^2(\mathbb{R}^3)$).

* However, mathematically it is not necessary for states to be wave fcts. Many results in quantum mechanics can be derived w/o referring to wave fcts. In fact there are systems (e.g. spin of pointlike particles) that are described by states in a Hilbert space w/o a wave fct. interpretation being available.

* Thus it is better to introduce an "abstract" Hilbert space $\mathcal{H}$ with "abstract" vectors ψ denoting states. From here on we will use the "ket" (*) notation for states: $|\psi\rangle$

(*) more on the motivation later.

IV.1.1 Bras and Kets

* Riesz Representation Theorem:

Let $F: \mathcal{H} \to \mathbb{C}$ be a linear complex-valued function (or 1-form) on $\mathcal{H}$.

Then there exists exactly one $|\psi_F\rangle \in \mathcal{H}$ such that $F(|\varphi\rangle) = \underbrace{\langle \psi_F | \varphi \rangle}_{\text{scalar product}}$

for all $|\varphi\rangle \in \mathcal{H}$.

I.e. 1 forms = scalar products with a certain vector.

* Conclusion: If F corresponds to the scalar product with a vector (or state)

$|\psi\rangle$ we denote $F = \langle \psi|$ ("bra notation")

Formally "bras" are dual vectors to kets. Finite-dimensional example:

kets = column vectors $\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$

bras = row vectors (a_1, a_2, a_3)

$\langle \text{bra} | \text{ket} \rangle = (\dots)\begin{pmatrix} \vdots \end{pmatrix}$ = scalar product

The bra-ket notation is consistent with and in fact motivated by the notation for the scalar product.

IV. 1.2. Representations

* Eigenstates of Hermitian operators play a particular role as bases. We will often use the eigenvalue of an eigenstate, or, if necessary, a complete set of eigenvalues of commuting operators, to uniquely label a state.

  Complete here means: we add commuting operators (i.e. with common eigenfunctions) until all degeneracies of eigenvalues are lifted.

  This is always possible, otherwise degenerate eigenfcts. would not be distinguishable by measurements.

* Examples:

  $|n\rangle$ = n^{th} eigenstate of harmonic osc.

  $|n_1, n_2, n_3\rangle$ for eigenstates of the 3-D infinite square well

  $|\vec{p}\rangle = |p_x, p_y, p_z\rangle$ for free (planar wave) eigenstates

  use eigenvalues of 3 operators p_x, p_y, p_z. Energy, e.g. alone would not be sufficient for labelling.

* Let $|a_i\rangle$, $i=1,..,N$ $N\in\mathbb{N}$ or $N=\infty$ be an orthonormal basis labelled by eigenvalues a_i (or sets thereof)

The amplitudes $\langle a_i|\psi\rangle$, $i=1,..,N$ define a Hilbert space which is isomorphic to the original space $\mathcal{H}$. $\langle a_i|\psi\rangle$ is called a representation of $|\psi\rangle$

The scalar product in the representation is $\langle\psi'|\psi\rangle \mapsto \sum_{i=1}^{N}\langle\psi'|a_i\rangle\langle a_i|\psi\rangle$

The value of the scalar product in the abstract space and the representation are the same since $\sum_{i=1}^{N}|a_i\rangle\langle a_i| = \mathbb{1}$ (closure relation)

(unity operator on $\mathcal{H}$)

Why? Follows from properties of bases.

* For basis labeled by continuous eigenvalue(s) $|c\rangle$, $c\in\mathbb{R}$ or a subset thereof:

$$\langle\psi'|\psi\rangle = \int dc\, \langle\psi'|c\rangle\langle c|\psi\rangle \quad \text{and} \quad \int dc\, |c\rangle\langle c| = \mathbb{1}$$

* Examples:

$\langle\vec{p}|\psi\rangle$ = amplitude for particle in state ψ to have momentum $\vec{p}$

= momentum-space wave fct. $\psi(\vec{p})$

analogous:

$\langle\vec{r}|\psi\rangle = \psi(\vec{r})$ coordinate space wave fct.

and for two states

$$\langle\psi|\psi\rangle = \int_{\mathbb{R}^3}\langle\psi'|\vec{r}\rangle\langle\vec{r}|\psi\rangle\, d^3r = \int_{\mathbb{R}^3}\psi^*(\vec{r})\,\psi(\vec{r})\, d^3r$$

consistent with wave mechanics formalism.

* Recall (properties of complex scalar products):

$\langle \varphi_1 | \varphi_2 \rangle = \langle \varphi_2 | \varphi_1 \rangle^*$

IV.1.3 Operators and Matrix Elements

* We will often write $\langle \varphi' | A | \varphi \rangle$ in bra-ket notation instead of $\underbrace{\langle \varphi' | A \varphi \rangle}_{\text{scalar product}}$ and interpret it as a matrix element of a matrix representation of the operator A.

* Generally, if the $|\varphi_i\rangle$ are an orthonormal basis of $\mathcal{H}$ we call the

$$\boxed{A_{ij} = \langle \varphi_i | A | \varphi_j \rangle} \qquad i,j \in 1,\dots,N$$

the matrix representation of A. This matrix encodes the full information about the operator A:

$$A|\varphi_j\rangle \underset{\text{closure}}{=} \sum_i |\varphi_i\rangle \langle \varphi_i | A | \varphi_j \rangle = \sum_i A_{ij} |\varphi_i\rangle$$

for any basis vector $|\varphi_j\rangle$

* Quantum mechanics can be completely cast in the form of these matrix elements.

E.g. let $|\phi\rangle = \sum_i a_i |\varphi_i\rangle$, $|\phi'\rangle = \sum_i b_i |\varphi_i\rangle$

Then $\langle\phi'|A|\phi\rangle = \sum_{ij} \underbrace{\langle\phi'|\varphi_i\rangle}_{b_i^*} \underbrace{\langle\varphi_i|A|\varphi_j\rangle}_{A_{ij}} \underbrace{\langle\varphi_j|\phi\rangle}_{a_j}$

$$= (b_1, \ldots, b_N)^* \begin{pmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \\ A_{N1} & \cdots & A_{NN} \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$$

* If the basis $|\varphi_i\rangle$ are eigenstates of the operator B then its matrix $B_{ij} = \lambda_i \delta_{ij}$ is diagonal and the λ_i are the eigenvalues.
* The operator $P_i = |\varphi_i\rangle\langle\varphi_i|$ is called the projection operator onto the basis state $|\varphi_i\rangle$.

Check: $P_i |\varphi_i\rangle = |\varphi_i\rangle$; $P_i |\varphi_j\rangle = |\varphi_i\rangle \underbrace{\langle\varphi_i|\varphi_j\rangle}_{=0} = \underset{\text{null state}}{0}$ for all $j \neq i$

Basic properties: $\sum_{i=1}^{N} P_i = \sum_{i=1}^{N} |\varphi_i\rangle\langle\varphi_i| = \mathbb{1}$ (closure)

$P_i^2 = P_i$ (check!)

* The matrix representation of the adjoint operator is the adjoint matrix.

$$(A^\dagger)_{ij} = A_{ji}^*$$

Why? $\langle\varphi_i|A^\dagger|\varphi_j\rangle = \langle A\varphi_i|\varphi_j\rangle = \langle\varphi_j|A\varphi_i\rangle^* = A_{ji}^*$

* We can formally define $|\psi\rangle^\dagger = \langle\psi|$ and obtain a consistent rule for the † operation:

$(A|\psi\rangle)^\dagger = \langle\psi|A^\dagger$ on the other hand $(A|\psi\rangle)^\dagger = |A\psi\rangle^\dagger = \langle A\psi|$

Prove they are equal by applying on arbitrary state $|\phi\rangle$:

$\langle\psi|A^\dagger|\phi\rangle = \langle A\psi|\phi\rangle$.

* The expectation value of A in a state $|\psi\rangle$ can now be written as a diagonal matrix element:

$$\langle A \rangle = \langle \psi | A | \psi \rangle .$$

* How can we get the operator A back from its matrix A_{ij}, $i,j = 1,\dots,N$?

$$A = \sum_{i,j=1}^{N} |\varphi_i\rangle A_{ij} \langle \varphi_j|$$

Why? $\sum_{i,j} |\varphi_i\rangle A_{ij} \langle\varphi_j| = \sum_{i,j} |\varphi_i\rangle\langle\varphi_i|A|\varphi_j\rangle\langle\varphi_j| = A$

* All statements in this chapter hold for uncountable Hilbert spaces with the usual replacement $\sum_i \to \int dc$

IV.1.4 Matrix Calculus Example: Plane Waves

* As an example we (re-)derive some basic results for coordinate space representation (for simplicity in 1 dimension).

We use $\langle x' | x \rangle = \delta(x'-x)$ and $\mathbb{1} = \int dx$

* For any analytic fct $f(x)$ of the position operator x: $\langle x'' | f(x) | x' \rangle = f(x')\,\delta(x''-x')$

Why? Clear. I.e. the matrix representing $f(x)$ is diagonal $(x''=x')$ with eigenvalues $f(x')$, since the $|x'\rangle$ are eigenfcts of operator x.

* $\langle x'' | p | x' \rangle = -i\hbar \frac{\partial}{\partial x''} \delta(x''-x')$ where p momentum operator.

Why? Recall that $p = -i\hbar \frac{\partial}{\partial x}$ in coordinate space but we won't use this.

We use the commutator $[x,p] = i\hbar$ as an algebraic postulate for these operators.

$\langle x'' | [x,p] | x' \rangle = i\hbar\, \delta(x''-x')$, on the other hand

$\langle x'' | xp - px | x' \rangle = (x''-x') \langle x'' | p | x \rangle$

Recall $x\, \delta'(x) = -\delta(x)$ (prove by integrating with a test fct.)

$\Rightarrow \langle x'' | p | x \rangle = -i\hbar \frac{\partial}{\partial x''} \delta(x''-x')$

* For momentum eigenstates in $\vec{r}$- representation

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p' x'}$$

Why? $\langle x'' | p | p' \rangle = \int dx' \langle x'' | p | x' \rangle \langle x' | p' \rangle = \int dx' (-i\hbar) \frac{\partial}{\partial x''} \delta(x''-x') \langle x' | p' \rangle$

$= -i\hbar \frac{\partial}{\partial x''} \langle x'' | p' \rangle$

but also $\langle x'' | p | p' \rangle = p' \langle x'' | p' \rangle$

$\Rightarrow \frac{\partial}{\partial x''} \langle x'' | p' \rangle = \frac{i}{\hbar} p' \langle x'' | p' \rangle \Rightarrow \langle x'' | p' \rangle = C\, e^{\frac{i}{\hbar} p' x''}$

Normalization: $\int \langle x'' | p' \rangle \langle p' | x' \rangle\, dp' = |C|^2 \int dp'\, e^{\frac{i}{\hbar} p' (x''-x')} = |C|^2\, 2\pi\hbar\, \delta(x''-x')$

$\underset{\text{but also}}{\parallel}$

$\langle x'' | x' \rangle = \delta(x''-x')$ $\Rightarrow |C|^2 = \frac{1}{2\pi\hbar}$

Note: we derived plane waves from purely algebraic considerations (in particular $[x,p]=i\hbar$) w/o using the Schrödinger equation at all.

IV.2 The Harmonic Oscillator Algebraically

* Without using the already known solutions we revisit the harm. osc. only using $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$ as the Hamiltonian and $[x,p] = i\hbar$.

* It turns out that the algebraic solution is better discussed in terms of two new operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + i \frac{p}{m\omega}\right)$$

$$a^+ = \sqrt{\frac{m\omega}{2\hbar}} \left(x - i \frac{p}{m\omega}\right) \qquad \text{(adjoint of } a\text{)}$$

Then $\boxed{H = \hbar\omega \left(a^+ a + \frac{1}{2}\right)}$ (check)

and $\boxed{[a, a^+] = \mathbb{1}}$ (i.e. a not Hermitian!)

Why? $[a, a^+] = \frac{m\omega}{2\hbar} \frac{+i}{m\omega} \Big(\underbrace{-xp + px - xp + px}_{-2i\hbar}\Big) = \mathbb{1}$

* a is called a lowering (annihilation) operator
a^+ " " raising (creation) operator

$a^+ a$ is called a number operator; it is Hermitian an commutes with H.

Label the common eigenstates of H and a^+a as $|\psi_n\rangle \equiv n$ with eigenvalues λ_n w.r.t. a^+a: $\quad a^+a|n\rangle = \lambda_n |n\rangle$, $\quad n \in \mathbb{N}$

$a^+|n\rangle$ is again an eigenvector of a^+a with eigenvalue $\lambda_n + 1$

Why? $a^+a(a^+|n\rangle) = a^+(a^+a + \mathbb{1})|n\rangle = (\lambda_n + 1) a^+ n$

Similarly: $a|n\rangle$ is an eigenstate of a^+a with eigenvalue $\lambda_n - 1$

$$\Rightarrow \quad a^\dagger|n\rangle = c_n|n+1\rangle \quad (1)$$

$$a|n\rangle = d_n\,|n-1\rangle \quad (2) \quad \text{if there is no degeneracy}$$

$(n\geq 1)$ see below

This justifies the "lowering", "raising" nomenclature

* The spectrum is bound from below by $\lambda_n \geq 0 \quad \forall n \in \mathbb{N}_0$

Why? $\langle n|a^\dagger a|n\rangle = \lambda_n \underbrace{\langle n|n\rangle}_{>0}$ and $\langle n|a^\dagger a|n\rangle = \underbrace{\langle an|an\rangle}_{>0}$

$\Rightarrow \lambda_n \geq 0.$

I.e. we have to modify (2) to be true only if $n\geq 1$.

Let us denote the ground state as $|0\rangle$ (note $|0\rangle \neq 0$)

Then $a^\dagger a|0\rangle = \lambda_0|0\rangle$ with $0\leq\lambda_0<1$ but also $a|0\rangle = 0$

$\Rightarrow \quad \lambda_0 = 0$

* Hence the eigenvalue spectrum of $a^\dagger a$ is ~~k~~ $0,1,2,\ldots = \mathbb{N}$

with eigenstates $|n\rangle = N_n (a^\dagger)^n|0\rangle \qquad n\in\mathbb{N}$; N_n = normalization

$\Rightarrow$ Stationary (energy eigenvalue) states are the same $|n\rangle$, $n\in\mathbb{N}$

and $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$

* This is a precursor to "second quantization" where "field quanta" are introduced. The quantum of the harmonic osc. that is created, annihilated or counted by $a^\dagger, a, a^\dagger a$, resp. is called a <u>phonon</u>.

* It is possible to reproduce the coordinate wave fcts. of the harmonic oscillator from this algebraic approach: $\langle \vec{r}, n \rangle = \psi_n(\vec{r})$

(maybe HW X)

IV.3 Simultaneous Measurement and Uncertainty

* Two observables represented by two operators A, B are called compatible, or simultaneously measureable, if they possess a common set of eigenstates with simultaneous eigenvalues (a_i, b_j), $i = 1, .., n$; $j = 1, .., m$ (n, m could be ∞)

The complete set of eigenstates can be labelled $|a_i, b_j\rangle$,

$$A|a_i, b_j\rangle = a_i |a_i, b_j\rangle \quad ; \quad B|a_i, b_j\rangle = b_j |a_i, b_j\rangle$$

(There might be degeneracies, as A, B might not be a complete set of operators).

* Theorem:

A, B simultaneously measureable

$$\Longleftrightarrow \quad [A, B] = 0$$

Why?

"$\Rightarrow$" A, B sim. measurable $\Rightarrow AB|a_i b_j\rangle = a_i b_j |a_i b_j\rangle = BA|a_i b_j\rangle$

for a complete basis $|a_i b_j\rangle \Rightarrow AB = BA$

"$\Leftarrow$" see Merzbacher, p. 215 ff

* Hence, conversely, if A, B do not commute, i.e.

$[A, B] = iC$ where $C \neq 0$ is an Hermitian (check!) operator,

then A, B can usually not be measured simultaneously with arbitrary precision. This can be quantified by an uncertainty relation between the variances $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle$, $(\Delta B)^2 = \langle (B - \langle B \rangle)^2 \rangle$ around the expectation values, similar to the one we already have for operators x and p.

* Theorem (Uncertainty Relation)

If $[A, B] = iC$ for Hermitian operators A, B, C then

$$\boxed{\Delta A \, \Delta B \geq \frac{1}{2} |\langle C \rangle|}$$

Why? Let $|\psi\rangle$ be the state in which the expectation values are evaluated.

$$(\Delta A)^2 = \langle \psi | (A - \langle A \rangle)^2 | \psi \rangle = \langle (A - \langle A \rangle)\psi | (A - \langle A \rangle)\psi \rangle = \| (A - \langle A \rangle)\psi \|^2$$

$$(\Delta B)^2 = \langle (B - \langle B \rangle)\psi | (B - \langle B \rangle)\psi \rangle = \| (B - \langle B \rangle)\psi \|^2$$

Recall Schwarz's inequality in Hilbert spaces: $\|\psi_a\|^2 \|\psi_b\|^2 \geq |\langle \psi_a | \psi_b \rangle|^2$

$$\Rightarrow (\Delta A)^2 (\Delta B)^2 \geq |\langle (A - \langle A \rangle)\psi | (B - \langle B \rangle)\psi \rangle|^2 = |\langle \psi | (A - \langle A \rangle)(B - \langle B \rangle)\psi \rangle|^2$$

We can write the operator on the right hand side as

$$(A-\langle A\rangle)(B-\langle B\rangle) = \frac{1}{2}\left[(A-\langle A\rangle)(B-\langle B\rangle)+(B-\langle B\rangle)(A-\langle A\rangle)\right] + \frac{1}{2}(AB-BA)$$

$$= \frac{1}{2}D + \frac{i}{2}C$$

Check: D Hermitian $\Rightarrow \langle D\rangle = \langle\psi|D|\psi\rangle \in \mathbb{R}$ real

and $\langle iC\rangle = i\langle\psi|C|\psi\rangle$ purely imaginary

$$\Rightarrow (\Delta A)^2(\Delta B)^2 \geq \left|\frac{1}{2}\langle D\rangle + \frac{i}{2}\langle C\rangle\right|^2 = \frac{1}{4}\left(\langle D\rangle^2 + \langle C\rangle^2\right) \geq \frac{1}{4}\langle C\rangle^2$$

q.e.d.

* Example: $[x,p] = i\hbar\,\mathbb{1} \Rightarrow C = \hbar\,\mathbb{1}$

$\Rightarrow \Delta x\,\Delta p \geq \frac{1}{2}\left|\langle\hbar\mathbb{1}\rangle\right| = \frac{\hbar}{2}$ same as already derived from wave mechanics in I.4