8 Hilbert space and matrix mechanics

8.1 Vector and linear function spaces

We alluded occasionally to analogy between vector spaces and abstract space of functions on which an inner product is defined. Now let's make this explicit.

Historically, quantum mechanics was really formulated 1st by Heisenberg in rather abstract way using obscure mathematical objects which (advisor) M. Born told him were matrices. Schrödinger's method developed 2nd, but gained wider acceptance, had immediate implications for wave-particle duality problem. Dirac showed two really same.

Analogy with ordinary linear algebra Denote Cartesian unit vectors by $\hat{\mathbf{r}}_i$, obey orthogonality relation

$$\hat{\mathbf{r}}_i \cdot \hat{\mathbf{r}}_j = \delta_{ij}, \tag{1}$$

can get ith component of a vector $\mathbf{A}$ by projecting,

$$A_i = \hat{\mathbf{r}}_i \cdot \mathbf{A}, \tag{2}$$

such that

$$\mathbf{A} = \sum_i A_i \hat{\mathbf{r}}_i = \sum_i (\hat{\mathbf{r}}_i \cdot \mathbf{A}) \hat{\mathbf{r}}_i. \tag{3}$$

The scalar product of 2 vectors is a *number*,

$$\mathbf{A} \cdot \mathbf{B} = \sum_i A_i B_i \tag{4}$$

While components of $\mathbf{A}$, namely A_x, A_y, A_z depend on coordinate system chosen (same vector in rotated coordinate system is A'_x, A'_y, A'_z), distances and scalar products are invariant under rotations, e.g.

$$\mathbf{A} \cdot \mathbf{B} = \mathbf{A}' \cdot \mathbf{B}' \tag{5}$$

Now think of wave function ψ describing quantum-mechanical state as vector in large space. Let $\{\psi_n\}$ be complete set of eigenstates of some observable. Can always arrange that ψ_n are orthogonal. Assume discrete e'values for now $\Longrightarrow$

$$(\psi_n, \psi_m) = \delta_{m,n} \tag{6}$$

(compare Eq. (1)). Completeness assumption is that any physically acceptable function ϕ can be expanded in terms of the ψ_n,

$$\phi = \sum_n c_n \psi_n, \tag{7}$$

which looks like Eq. (3). Expansion coefficients c_n thus completely specify state ϕ, can be thought of as components of vector. Inner product with $\chi = \Sigma_n d_n \psi_n$ is

$$(\phi, \chi) = \sum_{n,m} c_n^* d_m (\psi_n, \psi_m) = \sum_n c_n^* d_n \tag{8}$$

also a *number* like Eq. (4).

Suppose we have a *different* basis set of complete eigenfctns. $\{\eta_n\}$. Then the "components" of ϕ will look different in the new basis,

$$\phi = \sum_n c_n' \eta_n \tag{9}$$

but inner products will be invariant,

$$(\phi, \chi) = (\phi', \chi') \tag{10}$$

Continuous eigenvalues:

Suppose eigenfunctions ψ_q have *continuous* eigenvalue q, meaning no gaps between allowed values of q. Example to keep in the back of your mind: plane waves $\psi_p = e^{ipx}$ for infinite system.

Then orthogonality condition is

$$(\psi_q, \psi_q') = \delta(q - q'), \tag{11}$$

can expand

$$\phi = \int dq\; c(q)\psi_q \;;\; \chi = \int dq\; d(q)\psi_q \tag{12}$$

$$c(q) = (\phi, \psi_q) \;;\; d(q) = (\chi, \psi_q), \tag{13}$$

$$\text{and } (\phi, \chi) = \int dq\; c(q)^* d(q) \tag{14}$$

Although expressions involve integrals rather than discrete sums, formally analagous to discrete case: can regard ϕ as *vector* w/ components given by expansion coefficients.

8.2 Dirac's Bra ($\langle\psi|$) and Ket ($|\psi\rangle$) notation

- Physical system will now be described by vector in linear space ("Hilbert space"), written as

  $$|\psi\rangle, \quad |\phi\rangle, \quad |n, \ell, m\rangle, \ldots \tag{15}$$

  Might write particular eigenstate of H-atom as $|n, \ell, m\rangle$— letters simply *label* quantum state. Will also use

  $$|\mathbf{r}\rangle \text{ for single particle located at} \tag{16}$$

  $$\text{position } \mathbf{r} \quad (\star\ \textit{not}\ \psi(\mathbf{r})) \tag{17}$$

  $$|\mathbf{p}\rangle \text{ for particle with definite momentum } \mathbf{p} \tag{18}$$

- Space is *linear*:

  If $|\psi\rangle$, $|\phi\rangle$ elements of space, with α, β constants, then

  $$|\chi\rangle = \alpha|\psi\rangle + \beta|\phi\rangle \tag{19}$$

  is also an element of the space.

- Dual space:

  For every vector $|\psi\rangle$ we have an associated *dual* or *adjoint* vector $\langle\psi|$. In ordinary matrix algebra $|\psi\rangle$ may be thought of as column vector, $\langle\psi|$ as row vector!

- Inner product.

  For every pair $|\psi\rangle$, $\langle\phi|$ we assign complex no. $\langle\phi|\psi\rangle$ with following properties:

  1. $\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$

     $\boxed{\star \text{ Note this implies that the dual of } \alpha|\psi\rangle \text{ is } \alpha^*\langle\psi|.}$
  2. $\langle\phi|\phi\rangle$ real, > 0 unless $|\phi\rangle = 0$.
  3. linearity: $\langle\psi|(\alpha|\phi\rangle) = \alpha\langle\psi|\phi\rangle$,
     $\langle\psi|\left(\alpha|\phi\rangle + \beta|\chi\rangle\right) = \alpha\langle\psi|\phi\rangle + \beta\langle\psi|\chi\rangle$.

     N.B. Dual space is also linear

- Operators

  Linear operators in this space defined by

$$\hat{Q}|\psi\rangle = |\psi'\rangle, \tag{20}$$

  a new vector in Hilbert space. Linearity means

$$\hat{Q}\left(\alpha|\psi\rangle + \beta|\phi\rangle\right) = \alpha\hat{Q}|\psi\rangle + \beta\hat{Q}|\phi\rangle \tag{21}$$

  $\star$ All rules for addition and multiplication of operators hold as in Schrödinger representation.

- Operators on dual space

  This is a little tricky: action of operator $\hat{Q}$ on dual vector $\langle\psi|$ is

$$\langle\psi|\hat{Q} = \langle\psi'|, \tag{22}$$

also a vector in the dual space. Meaning of $\langle\psi'|$ is, for any $|\phi\rangle$,

$$\langle\psi'|\phi\rangle = \langle\psi|\ (\hat{Q}|\phi\rangle) \equiv \langle\psi|\hat{Q}|\phi\rangle \tag{23}$$

- Adjoint of operator

Def.:

$$\text{Dual of } \hat{Q}|\psi\rangle \text{ is } \langle\psi|\hat{Q}^\dagger \tag{24}$$

Frequently I'll be sloppy and write this as

$$(\ \hat{Q}|\psi\rangle\ )^\dagger = \langle\psi|\hat{Q}^\dagger \tag{25}$$

$\star$ All rules for adjoint we proved for S.-representation continue to hold, e.g.

$$(AB)^\dagger = B^\dagger A^\dagger \tag{26}$$

and

$$\langle\phi|\hat{Q}|\psi\rangle^* = \langle\psi|\hat{Q}^\dagger|\phi\rangle \tag{27}$$

- Eigenstates and eigenvalues

1. Eigenvalue eqn. for self-adjoint operator $\hat{Q}$ is
$$\hat{Q}|\psi\rangle = q|\psi\rangle \tag{28}$$

2. E'values of self-adjoint op. are real:
$$\begin{aligned} \langle\phi|\hat{Q}|\phi\rangle &= q\langle\phi|\phi\rangle \\ \langle\phi|\hat{Q}^\dagger|\phi\rangle &= q^*\langle\phi|\phi\rangle \end{aligned}$$
so $q = q^*$ if $\hat{Q} = \hat{Q}^\dagger$.

3. E'states belonging to different e'values are orthogonal:

   Assume

$$\begin{aligned} \hat{Q}|q_1\rangle &= q_1|q_1\rangle \\ \hat{Q}|q_2\rangle &= q_2|q_2\rangle \end{aligned}$$

   Then notice $\hat{Q}$ can act either to left or right:

$$\langle q_1|\hat{Q}|q_2\rangle = q_2\langle q_1|q_2\rangle \tag{29}$$

$$= q_1\langle q_1|q_2\rangle \tag{30}$$

   So if $q_1 \neq q_2$, must have $\langle q_1|q_2\rangle = 0$.

- Completeness:

  Any Hilbert space vector $|\psi\rangle$ can be expanded

$$|\psi\rangle = \sum_n c_n|n\rangle \tag{31}$$

  in terms of some complete set $|n\rangle >$ of e'states of some self-adj. operator $\hat{Q}$, e'values q_n assumed discrete for moment. The $|n\rangle >$ may be chosen orthonormalized,

$$\langle m|n\rangle = \delta_{mn} \tag{32}$$

  so expansion coeffs. c_n may be expressed (multiply Eq. (31) by $\langle m|$!)

$$c_n = \langle n|\psi\rangle \tag{33}$$

  or

$$|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle \tag{34}$$

$$= \left(\sum_n |n\rangle\langle n| \right) |\psi\rangle \tag{35}$$

So we can think of expression $\Sigma_n |n\rangle\langle n|$ as being a kind of operator, and from Eq. (35) we see it had better be the identity. This will be true if the $|n\rangle$ span the whole space, i.e. completeness means

$$\sum_n |n\rangle\langle n| = 1 \tag{36}$$

<u>continuous e'values</u>:

Orthogonality : $\langle q|q'\rangle = \delta(q - q')$,

similar arguments give

$$|\psi\rangle = \int dq\ |q\rangle\langle q|\psi\rangle \tag{37}$$

$$\Longrightarrow \int dq\ |q\rangle\langle q| = 1 \tag{38}$$

- Analogy with matrices, row and column vectors:

  Any state $|\psi\rangle$ specified completely by giving all the "components" $\langle n|\psi\rangle$ (see Eq. (34)).

  Same is true for state $\hat{Q}|\psi\rangle$:

$$\langle n|\hat{Q}|\psi\rangle = \sum_m \langle n|\hat{Q}|m\rangle\langle m|\psi\rangle \tag{39}$$

Now note this looks like a *matrix* equation relating *column vectors* $\langle n|\psi\rangle$ and $\langle n|\hat{Q}|\psi\rangle$:

$$\begin{pmatrix} \langle 1|\hat{Q}|\psi\rangle \\ \langle 2|\hat{Q}|\psi\rangle \\ \langle 3|\hat{Q}|\psi\rangle \\ \vdots \end{pmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & \cdots \\ Q_{21} & Q_{22} & Q_{23} & \cdots \\ Q_{31} & \cdots & & \\ \vdots & \vdots & & \end{bmatrix} \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \\ \vdots \end{pmatrix} \tag{40}$$

where the *matrix elements of the operator* $\hat{Q}$ are just

$$Q_{mn} = \langle m|\hat{Q}|n\rangle \tag{41}$$

Also since

$$\langle\psi|\hat{Q}|n\rangle = \sum_m \langle\psi|m\rangle\langle m|\hat{Q}|n\rangle, \tag{42}$$

can think of $\langle\psi|n\rangle$ and $\langle\psi|\hat{Q}|n\rangle$ as *row vectors*:

$$(\langle\psi|\hat{Q}|1\rangle \; \langle\psi|\hat{Q}|2\rangle \cdots) = (\langle\psi|1\rangle \; \langle\psi|2\rangle \cdots) \begin{bmatrix} Q_{11} & Q_{12} & \cdots \\ Q_{21} & Q_{22} & \cdots \\ \vdots & & \end{bmatrix} \tag{43}$$

Now we can make contact with the matrix algebra terminology, e.g. adjoint of matrix A specified by elements A_{mn} is mat. $A^\dagger$ with elements A^*_{nm}. For our self-adjoint observables $\hat{Q}$,

$$\begin{aligned} (Q_{mn})^* &= \langle m|\hat{Q}|n\rangle^* \\ &= \langle n|\hat{Q}^\dagger|m\rangle \\ &= \langle n|\hat{Q}|m\rangle \\ &= Q_{nm} \end{aligned} \tag{44}$$

In linear algebra such a matrix called Hermitian.

$$Q = Q^\dagger \equiv (Q^T)^* \tag{45}$$

- Relation to our friend the wavefunction

$|\mathbf{r}\rangle$ represents state with particle definitely at position $\mathbf{r}$. Note this provides continuous orthonormal basis:

$$\langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \tag{46}$$

In this basis state vector has "components"

$$
\begin{aligned}
\langle \mathbf{r}|\psi\rangle &\equiv \psi(\mathbf{r}) = \text{ Schrödinger's wavefctn} &(47)\\
\langle \psi|\mathbf{r}\rangle &= \psi^*(\mathbf{r}) &(48)
\end{aligned}
$$

so we can "expand" state $|\psi\rangle$ in this basis:

$$|\psi\rangle = \int d^3r|\mathbf{r}\rangle\langle\mathbf{r}|\psi\rangle = \int d^3r|\mathbf{r}\rangle\psi(\mathbf{r}) \tag{49}$$

Given 2nd state

$$|\phi\rangle = \int d^3r|\mathbf{r}\rangle\phi(\mathbf{r}) \tag{50}$$

we can take the inner product:

$$
\begin{aligned}
\langle\psi|\phi\rangle = \int d^3r d^3r' \langle\mathbf{r}'|\mathbf{r}\rangle\psi^*(\mathbf{r}') &= \int d^3r\psi^*(\mathbf{r})\phi(\mathbf{r})\\
&\equiv (\psi,\phi) &(51)
\end{aligned}
$$

to recover old notation explicitly!

- Time dependence

  Objective: "derive" Schrödinger eqn" from scratch! Pretend you are Heisenberg, and only know about state vectors in linear spaces. Given system is in state $|\psi(t_1)\rangle$, assume $|\psi(t_2)\rangle$ related to it by linear operator $\hat{U}$:

$$|\psi(t_2)\rangle = \hat{U}(t_2 - t_1)|\psi(t_1)\rangle \tag{52}$$

with $\hat{U}$ unitary, $\hat{U}\hat{U}^\dagger = 1$. For infinitesimal $\delta t = t_2 - t_1$, can Taylor expand:

$$\hat{U} = 1 - iH\delta t/\hbar, \tag{53}$$

So far don't know what H is really, merely plays role of 1st order Taylor coefficient in time evolution of $\hat{U}$ (did pull out factor of $\hbar$ to make sure it has dimensions of energy, however!) Now plug (53) into (52), rearrange:

$$\begin{aligned} \frac{|\psi(t_1+\delta t)\rangle - |\psi(t_1)\rangle}{\delta t} &= \frac{-iH|\psi(t_1)\rangle}{\hbar}, \text{ or} \\ i\hbar\frac{\partial|\psi\rangle}{\partial t} &= H|\psi\rangle \end{aligned} \tag{54}$$

which as we've said has formal solution

$$\hat{U}(t) = e^{-iHt/\hbar} \tag{55}$$

- Matrix mechanics $\longrightarrow$ wave mechanics

  sketch of Dirac's ideas:

  – Replace Poisson brackets in classical mechanics with commutators in quantum mechanics. Recall P.-bracket of two functions $f(q_i, p_i), g(q_i, p_i)$ of the coordinates q_i and momenta p_i in class. mech. defined by

  $$\{f, g\} \equiv \sum_i \left[\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right] \tag{56}$$

  With this definition, Newton's laws/ Hamilton's equations may be written generally as eqn. of motion for any fctn $f(q_i, p_i)$ (See any adv. class. mech. book):

  $$\frac{d}{dt}f = \{f, H\} \tag{57}$$

  e.g. take $f = p$, $H = p^2/2m + V(x)$, find

  $$dp/dt = -\partial V/\partial x \tag{58}$$

– What is starting point for sensible quantization procedure? 'Til now had guess for momentum operator based on free particle case, similar ad hoc guesses. Dirac: take as gospel commutation relations between operators, e.g. $\mathbf{p}, \hat{\mathbf{r}}$,

$$\star \qquad \text{replace } \{r_i, p_j\} = \delta_{ij} \to [\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}. \tag{59}$$

– Calculate matr. elts in $|\mathbf{r}\rangle$ basis of $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$:

$$\begin{aligned} \langle\mathbf{r}| \times \quad [\hat{r}_i, \hat{p}_j] &= i\hbar\delta_{ij} \quad \times |\mathbf{r}'\rangle \\ = (r_i - r_i')\langle\mathbf{r}|\hat{p}_j|\mathbf{r}'\rangle &= i\hbar\delta_{ij}\delta(\mathbf{r}-\mathbf{r}') \\ &= i\hbar(r_i - r_i')\frac{\partial}{\partial r_j}\delta(\mathbf{r}-\mathbf{r}') \end{aligned} \tag{60}$$

($\star$ last step a bit mysterious–exercise for reader!)

This says what $\mathbf{p}$ does to state $|\mathbf{r}\rangle$, therefore to $|\psi\rangle$:

$$\mathbf{p} = -i\hbar\nabla \tag{61}$$

as we found before by vague arguments about the free particle case, plane waves, etc. (see sec. 4).

– $H = \hat{p}^2/2m + V(\mathbf{r})$ is time evolution operator in sense of (55). **How do we know this?**

- Heisenberg representation

Choose orthonormal set of vectors $|n\rangle \equiv |n;0\rangle$ at time $t=0$. If we allow them to evolve according to Eq. (54), at a later time t they will be $|n;t\rangle$, with

$$|n;t\rangle = e^{-iHt/\hbar}|n;0\rangle \tag{62}$$

They'll still be a complete orthonormal set, though:

$$\begin{aligned}\langle n;t|m;t\rangle &= (\langle n|e^{iHt/\hbar})(e^{-iHt/\hbar}|m\rangle) \\ &= \langle n|m\rangle = \delta_{mn}\end{aligned} \tag{63}$$

so we could expand an arbitrary state vector $|\psi(t)\rangle$ in terms of these basis vectors with *constant coefficients*:

$$|\psi(t)\rangle = \sum_n c_n|n;t\rangle \tag{64}$$

In *Heisenberg rep.*, express everything in terms of $t-$ *independent* state functions $|\psi\rangle \equiv |\psi(0)\rangle$ (characterized by $|c_1, c_2 \ldots\rangle$.) Operators on other hand become $t-$ *dependent*, with matrix elements:

$$Q_{nm}(t) \equiv \langle n;t|\hat{Q}|n;t\rangle. \tag{65}$$

Time derivative of matrix:

$$\begin{aligned}\frac{d}{dt}\hat{Q} &= (\frac{\partial}{\partial t}\langle n;t|)\hat{Q}|n;t\rangle + \langle n;t|\hat{Q}\frac{\partial}{\partial t}|n;t\rangle \\ &= \frac{i}{\hbar}[H,\hat{Q}]\end{aligned} \tag{66}$$

Eq. (66) sometimes called Heisenberg eqn. of motion. Completely analogous to classical Poisson bracket equation, Eq. (57). **Thus without reference to specific form of "H", *canonical quantization* of Dirac tells us the mysterious time evolution operator "H" in Eq. (54) is the Hamiltonian of the system!**

$\Longrightarrow$ equivalence of matrix and wave mechanics.