Matrix Mechanics | Liboff chap. 11

Think back to discussions of the history of quantum mechanics. You recall that Schrödinger introduced his differential equation in the mid-late 20's, and put QM into a systematic form. You may also recall that at around the same time, Heisenberg came up with what turned out to be an equivalent formulation in terms of matrices.

It turns out the operators and wave fns of QM can be written as matrices and the equations can be written as matrix eq'ns. In fact we already have the concepts we need; it's simply a matter of putting them together properly. We already hinted at some of the ideas when we discussed representations of wave functions.

Here's how it works. We start with the idea of basis functions. Suppose we have a system with an associated wave fn ψ. which we can expand in terms of a discrete* set of basis functions $\{\varphi_n\}$

$$\psi = \sum_n a_n \varphi_n$$

* We'll talk about continuous systems later

The $\{\varphi_n\}$ might correspond to the energy eigenfns of the simple harmonic oscillator, say, or the particle in a box. So we can write

$$\psi = \sum_n \varphi_n a_n \qquad \text{with } a_n = \langle \varphi_n | \psi \rangle$$

$$\Rightarrow \quad |\psi\rangle = \sum_n |\varphi_n\rangle \langle \varphi_n | \psi \rangle \quad \text{in Dirac notation.}$$

The coeff's of this expansion, $a_n = \langle \varphi_n | \psi \rangle$, represent ψ in the representation where $\{\varphi_n\}$ is the basis (the a_n are projections of ψ onto the basis vectors φ_n).

$\Rightarrow$ The $\{a_n\}$ are equivalent to ψ: knowing the $\{a_n\}$ (and the basis) completely specifies ψ.

So we can imagine ψ as a column vector whose components are the a_n:

$$\psi = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}$$

$$\left[\text{Ex: } \psi = \frac{1}{\sqrt{3}} \varphi_1 + \sqrt{\frac{2}{3}} \varphi_3 \Rightarrow \psi \rightarrow \begin{pmatrix} \frac{1}{\sqrt{3}} \\ 0 \\ \frac{2}{\sqrt{3}} \\ 0 \\ 0 \\ \vdots \end{pmatrix} \right]$$

Now what about operators? We want to be able to write operator eq'ns. Let F be an arbitrary operator, and let ψ + ψ' be some wave functions, where we have the QM eq'n (8.3)

$$\psi = F\psi' \qquad (*)$$

or $$|\psi\rangle = F|\psi'\rangle$$

We can write $|\psi'\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi'\rangle$, + substituting,

$$|\psi\rangle = \sum_n F|\varphi_n\rangle\langle\varphi_n|\psi'\rangle$$

Now let's multiply on the left with $\langle\varphi_q|$:

$$\underbrace{\langle\varphi_q|\psi\rangle}_{a_q} = \sum_n \underbrace{\langle\varphi_q|F|\varphi_n\rangle}_{\equiv F_{qn}}\underbrace{\langle\varphi_n|\psi'\rangle}_{a_n'}.$$

or $$a_q = \sum_n F_{qn}a_n' \qquad (**)$$

and $$\boxed{F_{qn} \equiv \langle\varphi_q|F|\varphi_n\rangle = \int \varphi_q^* F \varphi_n \, d^{(3)}x}$$

is the matrix representation of the operator F →

in this basis $\{\varphi_n\}$, also known as the qn matrix element of F.

So the operator eq'n (*) has become the matrix eq'n (**). Written out explicitly, we have

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} F_{11} & F_{12} & \cdots \\ F_{21} & F_{22} & \\ \vdots & & \end{pmatrix} \begin{pmatrix} a_1' \\ a_2' \\ \vdots \\ \vdots \end{pmatrix}$$

<u>Diagonalization</u> of an operator:

Suppose the basis vectors are eigenvectors of an operator G (e.g. energy eigenstates + Hamiltonian):

$$G\varphi_n = g_n \varphi_n$$

The matrix elements of G are

$$G_{qn} = \langle \varphi_q | G | \varphi_n \rangle = \langle \varphi_q | g_n | \varphi_n \rangle = g_n \langle \varphi_q | \varphi_n \rangle$$
$$= g_n \delta_{qn}$$

$$\Rightarrow G_{qn} = g_n \delta_{qn} = \begin{pmatrix} g_1 & 0 & 0 & \\ 0 & g_2 & 0 & \cdots \\ & & g_3 & \\ 0 & & & \ddots \\ \vdots & & & \end{pmatrix}$$

$\Rightarrow G$ is diagonal. The matrix of an operator in a basis of its eigenfns is diagonal. (8.5)

The eigenfns take on a simple form too:

$$|\psi_n\rangle = \sum_q a_q^n |\psi_q\rangle$$

$$\text{but } a_q^n = \langle\psi_n|\psi_q\rangle = \delta_{nq}$$

$$\Rightarrow a_q^n = \delta_{nq}$$

$$\psi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad \psi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \ldots \psi_n = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

So the eigenvalue eq'n becomes

$$\sum_q \langle\psi_p|G|\psi_q\rangle\langle\psi_q|\psi_n\rangle = g_n\langle\psi_p|\psi_n\rangle$$

which looks in matrix form like, e.g.

$$\begin{pmatrix} g_1 & & \textcircled{0} & \\ & g_2 & \cdots & \\ 0 & & g_3 & \\ & \ddots & & \ddots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = g_3 \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

Now for a generic vector the normalization is

$$|\psi|^2 = \langle\psi|\psi\rangle = \sum \langle\psi|\varphi_q\rangle\langle\varphi_q|\psi\rangle$$

$$= \sum_q |a_q|^2$$

and in an orthonormal basis

$$|\varphi_n|^2 = \sum_q |a_q^n|^2 = 1$$

and in matrix form

$$|\varphi_n|^2 = (0 \cdots 1 \cdots 0)\begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = 1$$

Now, we can show (see book p. 485) that if G is diagonal in a particular basis, then that basis is made of eigenfns of G.

$\Rightarrow$

Finding eigenvalues of an operator

$\Longleftrightarrow$

finding a basis which diagonalizes the operator

And: Complete set of commuting operators $\Leftrightarrow$ common eigenfns $\Leftrightarrow$ $\exists$ representation in which matrices corresp. to all of the op's in set are diagonal.

Continuous case: indices range over continuum of values e.g. free particle. Hamiltonian looks like

$$\langle k | H | k' \rangle = \langle k | \frac{p_k^2}{2m} | k' \rangle = \frac{\hbar^2 k'^2}{2m} \delta(k-k')$$

Kronecker $\delta \rightarrow$ Dirac δ

and matrix eq'ns still look like differential eq'ns.

<u>Properties of Matrices</u>: see pp. 488–490 for properties of matrices. Notation: often use ^{T} for transpose:

$$A^T_{ij} = A_{ji}$$

Hermitian conjugate: $A^+ = (A^T)^*$

A Hermitian $\Rightarrow$ $A^{*T} = A$

+ if diagonal, $A^* = A$ $\Rightarrow$ Hermitian op's have real eigenvalues

TABLE 11.1 Matrix properties

Matrix	Definition	Matrix Elements
Symmetric	$A = \tilde{A}$	$A_{pq} = A_{qp}$
Antisymmetric	$A = -\tilde{A}$	$A_{pp} = 0$; $A_{pq} = -A_{qp}$
Orthogonal	$A = \tilde{A}^{-1}$	$(\tilde{A}A)_{pq} = \delta_{pq}$
Real	$A = A^*$	$A_{pq} = A_{pq}{}^*$
Pure imaginary	$A = -A^*$	$A_{pq} = iB_{pq}$; B_{pq} real
Hermitian	$A = A^\dagger$	$A_{pq} = A_{qp}{}^*$
Anti-Hermitian	$A = -A^\dagger$	$A_{pq} = -A_{qp}{}^*$
Unitary	$A = (A^\dagger)^{-1}$	$(A^\dagger A)_{pq} = \delta_{pq}$
Singular	$\det A = 0$	

Simple Harmonic Oscillator — Matrix Formulation (8.8)

As an example, we can write the simple harmonic oscillator in matrix form,

We will use the energy representation, in which the Hamiltonian matrix is diagonal. Our basis states are then eigenfns of the hamiltonian:

$$H\psi_n = E_n\psi_n \qquad H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2$$

$$\{\psi_n\} = e^{-\xi^2/2}\{A_0\mathcal{H}_0(\xi),\ A_1\mathcal{H}_1(\xi),\ \ldots\} = \{|0\rangle, |1\rangle, |2\rangle, \ldots\}$$

$$\xi^2 = \beta^2 x^2 \qquad \beta^2 = \frac{m\omega_0}{\hbar}$$

and $\mathcal{H}_n(\xi)$ are the Hermite polynomials.

$$E_n = \hbar\omega_0(n + 1/2)$$

In matrix rep., we have

$$|0\rangle = \begin{pmatrix}1\\0\\0\\0\\\vdots\end{pmatrix} \qquad |1\rangle = \begin{pmatrix}0\\1\\0\\0\\\vdots\end{pmatrix} \qquad |2\rangle = \begin{pmatrix}0\\0\\1\\0\\\vdots\end{pmatrix}$$

$$H = \hbar\omega_0\begin{pmatrix}1/2 & & & & 0\\ & 3/2 & & & \\ & & 5/2 & & \\ & & & \ddots & \\ 0 & & & & n+\frac{1}{2}\end{pmatrix}$$

Now what about the position and momentum op's? We know the energy eigenstates are <u>not</u> eigenstates of position + momentum (i.e., x + p don't commute w/ H), so we don't expect the corresp. matrices to be diagonal.

To find x + p matrix elements, it's easiest to write them in terms of the raising & lowering ops, a^+ + a.

Recall (cf pp. 6.7ff + esp. p. 6.16)

$$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$
$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

So $\quad a_{nk} = \langle n|\hat{a}|k\rangle = \sqrt{k}\,\langle n|k-1\rangle = \sqrt{k}\,\delta_{n,k-1}$

$$\Rightarrow \quad a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 \cdots \\ & \cdots & & & \end{pmatrix}$$

and $\quad a^+_{nk} = \langle n|a^+|k\rangle = \sqrt{k+1}\,\delta_{n,k+1}$

$$a^+ = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 \cdots \\ 0 & 0 & \sqrt{3} & 0 \cdots \\ & \vdots & & \end{pmatrix}$$

And you can check that $a^+|n\rangle$ + $a|n\rangle$ in matrix rep. really do what they claim to do.

Getting back to position and momentum, recall (8.10)
from the original def's of a + a^+ we can write

$$x = \frac{1}{\sqrt{2}\beta}(a + a^+) \qquad p = \frac{m\omega_0}{\sqrt{2}i\beta}(a - a^+)$$

So to get the matrix elements,

$$\langle n|x|k\rangle = \frac{1}{\sqrt{2}\beta}\left[\sqrt{k}\,\delta_{n,k-1} + \sqrt{k+1}\,\delta_{n,k+1}\right]$$

$$x = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \\ & & \vdots & & \end{pmatrix}$$

Similarly

$$\langle n|p|k\rangle = \frac{m\omega_0}{\sqrt{2}i\beta}\left[\sqrt{k}\,\delta_{n,k-1} - \sqrt{k-1}\,\delta_{n,k+1}\right]$$

$$p = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \vdots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & -\sqrt{3} & 0 & \cdots \\ & \vdots & & & \end{pmatrix}$$

and notice that both matrices (x + p) are hermitian.

Finally, how about the number operator $N = a^\dagger a$? (8.11)

If we multiply the $a^\dagger$ & a matrices, we get

$$N = \begin{pmatrix} 0 & & & & & \\ & 1 & & & 0 & \\ & & 2 & & & \\ & & & 3 & & \\ & 0 & & & \ddots & \\ & & & & & n \\ & & & & & & \ddots \end{pmatrix}$$

as we would expect.

Pauli Spin Matrices - spin-$\frac{1}{2}$ particles

Spin is an angular momentum, so it satisfies

$$[S_x, S_y] = i\hbar S_z \; ; \; [S_y, S_z] = i\hbar S_x \; ; \; [S_z, S_x] = i\hbar S_y$$

and raising and lowering operators

$$S_\pm = S_x \pm i S_y \quad \text{with } S_\pm |s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}\; |s, m_s \pm 1\rangle$$

Eigenvalue eq'ns

$$S^2 |s m_s\rangle = \hbar^2 s(s+1) |s m_s\rangle \qquad S_z |s m_s\rangle = \hbar m_s |s m_s\rangle$$

Now let's talk about spin $\frac{1}{2}$, which covers electrons, protons, neutrons, and quarks.

We want the matrix representation with S^2 + S_z diagonal.

Well, there are two ways to go. One, done in the book, is to postulate eigenstates α + β w/ $S_z = \frac{\hbar}{2}$ + $S_z = -\frac{\hbar}{2}$ respectively, and to use the above eq'ns to solve for all the matrix elements.

Another approach is to start from S_z; It is diagonal w/ eigenvalues $+\frac{\hbar}{2}$ + $-\frac{\hbar}{2}$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and eigenvectors $\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Then use the raising & lowering op's to find the matrix elements of S_y & S_z.

We find $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

We can therefor write

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

Where $\vec{\sigma}$ are the Pauli spin matrices, w/

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that they're hermitian.

The eigenvectors, and their linear combinations which are spin wave fns for spin ½ particles, are called "spinors"

The mathematics describing interactions involving spin (such as a spin in a magnetic field) use the Pauli spin matrices.

Magnetic moment $\vec{\mu} = \frac{e}{mc}\vec{S} = \frac{e\hbar}{2mc}\vec{\sigma}$