Think back to discussions of the history of quantum mechanics. You recall that Schrödinger introduced his equation in the mid-1920s, 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 functions of QM can be written as matrices and the equations can be written as matrix eqns. 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 function \( \Psi \), which we can expand in terms of a discrete set of basis functions \( |\psi_n\rangle \)

\[ \Psi = \sum_n a_n |\psi_n\rangle \]

We'll talk about continuous systems later...
The \( \xi n \) might correspond to the energy eigenfuns of the simple harmonic oscillator, say, or the particle in a box. So we can write

\[
\psi = \sum_n \xi_n \alpha_n \quad \text{with} \quad \alpha_n = \langle \phi_n | \psi \rangle
\]

\[\Rightarrow \quad |\psi\rangle = \sum_n \xi_n |\phi_n\rangle \langle \phi_n | \psi \rangle \quad \text{in Dirac notation.}\]

The coff's of this expansion, \( \alpha_n = \langle \phi_n | \psi \rangle \), represent \( \psi \) in the representation where \( \xi \phi_n \) is the basis (the \( \alpha_n \) are projections of \( \psi \) onto the basis vectors \( \phi_n \)).

\[\Rightarrow \quad \xi \phi_n \text{ are equivalent to } \psi: \text{ knowing the } \xi \phi_n \text{ (and the basis) completely specifies } \psi.\]

So we can imagine \( \psi \) as a column vector whose components are the \( \alpha_n \):

\[
\psi = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}
\]

\[\text{Ex: } \psi = \frac{1}{\sqrt{3}} \phi_1 + \sqrt{2/3} \phi_3 \Rightarrow \psi \rightarrow \begin{pmatrix} 1/3 \\ 0 \\ \sqrt{2/3} \end{pmatrix}\]
Now what about operators? We want to be able to write operator eqn's. Let $\hat{F}$ be an arbitrary operator, and let $\Psi$ and $\Psi'$ be some wave functions, where we have the QM eq'n

$$\Psi = \hat{F} \Psi' \quad (\star)$$

or

$$\Psi' = \hat{F} \Psi$$

We can write $\Psi' = \sum_n |\Psi_n\rangle \langle \Psi_n| \Psi' \rangle$, and substituting,

$$\Psi = \sum_n \hat{F} |\Psi_n\rangle \langle \Psi_n| \Psi' \rangle$$

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

$$\langle \Psi_n| \Psi \rangle = \sum_n \langle \Psi_n| \hat{F} |\Psi_n\rangle \langle \Psi_n| \Psi' \rangle$$

or

$$a_q = \sum_n F_{qn} a_n' \quad (\star \star)$$

and

$$F_{qn} = \langle \Psi_n| \hat{F} |\Psi_q\rangle = \int \Psi_q^* \hat{F} \Psi_n \, d^3x$$

is the matrix representation of the operator $\hat{F}$.
in this basis \( \{ \Phi_n \} \), also known as the matrix element of \( a^n \).

So the operator eqn (\*) has become the matrix eqn (\**). Written out explicitly, we have

\[
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
\end{pmatrix} =
\begin{pmatrix}
a_1' \\
a_2' \\
\vdots \\
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
\end{pmatrix}
\]

**Diagonalization of an operator:**

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

\[
G \Phi_n = g_n \Phi_n
\]

The matrix elements of \( G \) are

\[
G_{mn} = \langle \Phi_m | G | \Phi_n \rangle = \langle \Phi_n | G | \Phi_n \rangle = g_n \langle \Phi_m | \Phi_n \rangle = g_n \delta_{mn}
\]

\[
\Rightarrow G_{mn} = g_n \delta_{mn} = \begin{pmatrix}
g_1 & 0 & 0 \\
0 & g_2 & 0 \\
0 & 0 & g_3 \\
\end{pmatrix}
\]
A $\Lambda$ is diagonal. The matrix of an operator in a basis of its eigenfunctions is diagonal.

The eigenfunctions take on a simple form too:

$$|\Psi_n\rangle = \frac{3}{2} a_n^* |\Psi_q\rangle$$

but $a_n^* = \langle \Psi_n | \Psi_q \rangle = \delta_{nq}$

$$\Rightarrow a_n^* = \delta_{nq}$$

$$|\Psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad |\Psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \quad \cdots \quad |\Psi_n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \end{pmatrix}$$

So the eigenvalue equation becomes

$$\sum_{q} <\Psi_p|\Lambda|\Psi_q><\Psi_q|\Psi_n> = g_n <\Psi_p|\Psi_n>$$

which looks in matrix form like, e.g.

$$\begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} = g_n \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}$$
Now for a generic vector the normalization is

\[ |\psi|^2 = \langle \psi | \psi \rangle = \sum_q |\langle \psi_q | \psi \rangle|^2 = \sum_q |\psi_q|^2 \]

and in an orthonormal basis,

\[ |\psi_n|^2 = \sum_q |\psi_q|^2 = 1 \]

and in matrix form,

\[ |\psi_n|^2 = (0 \cdots 1 \cdots 0) \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \end{pmatrix} = 1 \]

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

Finding eigenvalues of an operator

\[ (\Rightarrow \quad \text{finding a basis which diagonalizes the operator}) \]

And: Complete set of commuting operators \((\Rightarrow \quad \text{common eigenfns})\) \( \Rightarrow \) representation in which matrices corresponding to all of the cp's in set are diagonal.
Continuous case: indices range over continuum of values e.g., free particle. Hamiltonian looks like

\[ \langle K | H | K' \rangle = \langle k | \frac{p^2}{2m} | k' \rangle = \frac{\hbar^2}{2m} \delta(k-k') \]

Kronecker \( \delta \to \) Dirac \( \delta \)

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

Properties of Matrices: see pp. 488-490 for properties of matrices. Notation: often use \( \text{T} \) for transpose:

\[ A_{ij}^T = A_{ji} \]

Hermitian conjugate: \( A^* = (A^\text{T})^* \)

\( A \) Hermitian \( \Rightarrow \) \( A^* \text{T} = A \)

\( \oplus \) if diagonal, \( A^* = A \Rightarrow \) Hermitian op's have real eigenvalues.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Definition</th>
<th>Matrix Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetric</td>
<td>( A = \overline{A} )</td>
<td>( A_{pq} = A_{qp} )</td>
</tr>
<tr>
<td>Antisymmetric</td>
<td>( A = -\overline{A} )</td>
<td>( A_{pp} = 0; A_{pq} = -A_{qp} )</td>
</tr>
<tr>
<td>Orthogonal</td>
<td>( A = A^{-1} )</td>
<td>( (A\overline{A})<em>{pq} = \delta</em>{pq} )</td>
</tr>
<tr>
<td>Real</td>
<td>( A = A^* )</td>
<td>( A_{pq} = A_{qp} )</td>
</tr>
<tr>
<td>Pure imaginary</td>
<td>( A = -A^* )</td>
<td>( A_{pq} = iB_{pq}; B_{pq} \text{ real} )</td>
</tr>
<tr>
<td>Hermitian</td>
<td>( A = A^\dagger )</td>
<td>( A_{pq} = A_{qp}^* )</td>
</tr>
<tr>
<td>Anti-Hermitian</td>
<td>( A = -A^\dagger )</td>
<td>( A_{pq} = -A_{qp}^* )</td>
</tr>
<tr>
<td>Unitary</td>
<td>( A = (A^\dagger)^{-1} )</td>
<td>( (A^\dagger A)<em>{pq} = \delta</em>{pq} )</td>
</tr>
<tr>
<td>Singular</td>
<td>( \det A = 0 )</td>
<td></td>
</tr>
</tbody>
</table>
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:

\[ H \psi_n = E_n \psi_n \quad \quad H = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 x^2 \]

\[ \varepsilon \psi_n \psi_m = e^{-\frac{\varepsilon^2}{2}} \sum A_n(x) \psi_m \psi_m, A_n(x), \ldots \varepsilon \in \{0, 1, 2, \ldots \} \]

\[ \varepsilon^2 = \beta^2 \omega_0^2 \quad \beta = \frac{m \omega_0}{2} \]

and \( H_n(x) \) are the Hermite polynomials.

\[ E_n = \hbar \omega_0 (n + \frac{1}{2}) \]

In matrix rep., we have:

\[ |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \ldots \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \ldots \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \ldots \end{pmatrix} \]

\[ H = \hbar \omega_0 \begin{pmatrix} \frac{3}{2} & \frac{1}{2} & \ldots \\ \frac{1}{2} & \frac{3}{2} & \frac{1}{2} \ldots \\ \ldots & \ldots & \ldots \\ \Omega & \frac{1}{2} & \frac{3}{2} \ldots \\ 0 & \Omega & \frac{1}{2} \ldots \\ 0 & 0 & \Omega \ldots \end{pmatrix} \]
Now what about the position and momentum operators? We know the energy eigenstates are not eigenstates of position and momentum (i.e., x and p don’t commute w/ H), so we don’t expect the corresponding matrices to be diagonal.

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

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

\[
\begin{align*}
|n\rangle &= \sqrt{n} \, |n-1\rangle \\
|n+1\rangle &= \sqrt{n+1} \, |n\rangle
\end{align*}
\]

So \( a^k |n\rangle = \sqrt{k} |n\rangle \) and \( a |k\rangle = \sqrt{k} \, |k-1\rangle = \sqrt{k} \, \delta_{n,k-1} \)

\[
\Rightarrow \quad a = \begin{pmatrix}
0 & \sqrt{1} & 0 & 0 & \cdots \\
0 & 0 & \sqrt{2} & 0 & \cdots \\
0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots
\end{pmatrix}
\]

and \( a^k |n\rangle = \sqrt{k+1} \, \delta_{n,k+1} \)

\[
\begin{align*}
a^+ &= \begin{pmatrix}
0 & 0 & 0 & \cdots \\
0 & \sqrt{1} & 0 & 0 & \cdots \\
0 & 0 & \sqrt{2} & 0 & \cdots \\
0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots
\end{pmatrix}
\end{align*}
\]

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 from the original def's of $a + a^+$ we can write

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

So to get the matrix elements,

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

$$x = \frac{1}{\sqrt{2i\beta}} \begin{pmatrix} 0 & \sqrt{5} & 0 & 0 & \cdots \\ \sqrt{5} & 0 & \sqrt{15} & 0 & \cdots \\ 0 & \sqrt{15} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Similarly

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

$$p = \frac{m\omega_0}{\sqrt{2i\beta}} \begin{pmatrix} 0 & \sqrt{5} & 0 & 0 & \cdots \\ -\sqrt{5} & 0 & \sqrt{15} & 0 & \cdots \\ 0 & -\sqrt{15} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

and notice that both matrices $(x+p)$ are hermitian.
Finally, how about the number operator $N = a^+ a$? If we multiply the $a^+ + a$ matrices, we get

$$N = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

as we would expect.
Pauli Spin Matrices - spin 1/2 particles

Spin is an angular momentum, so it satisfies

\[ [S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_y] = i\hbar S_x. \]

and raising and lowering operators

\[ S_+ = S_x + iS_y \quad \text{with} \quad S_\pm |s, m_s\rangle = \sqrt{s(s+1) - m_s(m_s \pm 1)} |s, m_s \pm 1\rangle \]

Eigenvalue eqns

\[ s^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle \quad S_z^2 |s, m_s\rangle = \hbar m_s |s, m_s\rangle \]

Now let's talk about spin 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 \( \alpha + \beta \) w/ \( S_z = \frac{1}{2} \) respectively, and to use the above eqns to solve for all the matrix elements.

Another approach is to start from \( S_z \) itself being diagonal w/ eigenvalues \( \pm \frac{1}{2}, -\frac{1}{2} \)

\[ S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

and eigenvectors \( \alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \).
Then use the raising & lowering operators to find the matrix elements of $S_\hat{x}$ & $S\hat{z}$.

We find

$$S_x = \frac{h}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

We can therefore write

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

Where $\hat{\sigma}$ are the Pauli spin matrices, with

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

Note that they're hermitian.

The eigenvectors, and their linear combinations, which are spin wave fits for spin $1/2$ particles, are called "spinors".

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

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