The quantum state as a vector

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1 Wave mechanics

In our review of the development of wave mechanics, we have established several basic properties of the quantum description of nature:

1. A particle (perhaps better viewed as a "quantized field") may be described by a complex function, called the wave function, $\psi(\mathbf{x}, t)$, which contains information about what can be measured concerning the particle.

2. We normalize ψ so that the integral of the norm over all space is one:

$$\int_{all\ space} \psi^* \psi d^3x = 1$$

   This allows us to interpret

$$\psi^* \psi d^3x$$

   as the probability of finding the particle in the infinitesimal volume, d^3x. The product $\psi^*\psi$ is then a probablility density.

3. There are various Hermitian linear operators for dynamical variables, also called physical observables, such as position, energy and momentum. These three are given by

$$\begin{aligned} \hat{\mathbf{x}} &= \mathbf{x} \\ \hat{E} &= i\hbar \frac{\partial}{\partial t} \\ \hat{\mathbf{p}} &= -i\hbar \boldsymbol{\nabla} \end{aligned}$$

4. Measurement of a dynamical variable always yields an eigenvalue of the corresponding linear operator, and changes the state to the corresponding eigenvector. It is modeled by allowing the operator corresponding to the dynamical variable act on the wave function.

5. Between measurements, the state evolves according to the Schrödinger equation.

6. We can describe spin-$\frac{1}{2}$ systems as 2-component vectors, $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$, where the α-component is the degree of "spin up" and the β-component the degree of "spin down".

We now introduce notation which is general enough to encompass both the spin and the wave function, and at the same time allows us the full symmetry of phase space in choosing the basis.

The central observation to be made is that both 2-component spinor, and wave functions ψ, are vectors in a vector space. This is clear for the 2-component spinors, but observe that normalizable functions also

form a vector space since we may take linear combinations and use the distributive laws. Thus, if ψ_1 and ψ_2 are two normalizable complex functions, then the linear combination

$$\alpha\psi_1 + \beta\psi_2$$

is also. We have the distributive laws,

$$\begin{aligned} (\alpha + \beta)\,\psi &= \alpha\psi + \beta\psi \\ \alpha\,(\psi_1 + \psi_2) &= \alpha\psi_1 + \alpha\psi_2 \end{aligned}$$

It is straightforward to check that all of the criteria of a vector space (see "More than you need to know on Vector Spaces" are satisfied by functions. The vector space of quantum mechanics is required to have a norm, in this case, $\psi^*\psi$, and be complete. Completeness is the statement that linear combinations of vectors also lie in the vector space.

2 Kets and Bras

We now define a new symbol for a vector, called the *ket*:

$$|\ >$$

Kets are usually written with a label inside, chosen for our convenience to remind us what particular vector we are interested in. Thus, a spin up eigenstate of the operator for the x-component of angular momentum might be written as

$$|x, +>$$

while the spin down eigenstate might be

$$|x, ->$$

To generalize our notion of wave function, we may write

$$|\psi>$$

There is an important difference between a ket, and the wave function. The ket represents a formal vector in an infinite dimensional space, whereas the wave function is the vector in a particular basis. Similarly, our spin state kets are formal vectors in a 2-dimensional space, whereas the spinor

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

is the state vector in a particular basis. To make this difference clear, we introduce a basis for spin states. Let the z-eigenkets be denoted simply

$$|+>$$
$$|->$$

For eigenstates along a general direction, $\hat{\mathbf{n}}$, other than z, we write the eigenstates as

$$|\hat{\mathbf{n}}, \pm>$$

In a normed vector space, there are always two kinds of vector. One way to see this is to think of the collection of all linear maps from the first vector space (here, the space of kets) to the real or complex numbers:

$$\phi : \{|\psi>\} \to \mathcal{C}$$

Since linear combinations of linear maps are still linear maps, such maps form a vector space. We denote an element of this second vector space by a reversed ket, called a *bra*,

$$< \phi|$$

and write the mapping as a *bra-ket*, dropping one of the middle bars to form a bracket

$$< \phi||\psi > \quad = \quad < \phi|\psi > \in \mathcal{C}$$

that is, $< \phi|\psi >$ is the complex number that results when the linear map ϕ acts on the vector $|\psi >$.

We may think of bras and kets as completely equivalent vector spaces, since we could just as easily have taken $|\psi >$ to be a linear map from the vector space of bras to the complex numbers. The vector spaces are generalizations of the wave function and its conjugate:

$$\begin{array}{rcl} \psi & \rightarrow & |\psi > \\ \phi^* & \rightarrow & < \phi| \end{array}$$

Indeed, the inner product of wave functions is $\phi^*\psi \rightarrow < \phi|\psi >$, and from this we are motivated to require that

$$< \psi|\phi > \quad = \quad < \phi|\psi >^*$$

With this in mind, associated with any give ket, there is a unique bra,

$$< \psi| \quad \longleftrightarrow \quad |\psi >$$

3 Bases

We know that any vector may be written as a linear combination of a set of basis vectors, defined as any minimal set of linearly independent vectors. For example, in the 2-dimensional space of spinors, any two independent vectors form a basis. Let the eigenvectors of the z-component of angular momentum be taken as our basis for spinors. Then we may write any other spin ket as a linear combination,

$$|\alpha > \quad = \quad a|+ > \, + b|- >$$

We can find the values of a and b using maps. Find the dual bras for the basis,

$$\begin{array}{rcl} |+ > & \rightarrow & < +| \\ |- > & \rightarrow & < -| \end{array}$$

Then acting from the left with each of these, we have

$$\begin{array}{rcl} < +|\alpha > & = & a < +|+ > \, + b < +|- > \\ & = & a \end{array}$$

since the basis kets are orthogonal,

$$\begin{array}{rcl} < +|+ > & = & < -|- >= 1 \\ < +|- > & = & < -|+ >= 0 \end{array}$$

Similarly,

$$\begin{array}{rcl} < -|\alpha > & = & a < -|+ > \, + b < -|- > \\ & = & b \end{array}$$

This means that the original ket may be expanded as

$$|\alpha> \;=\; (<+|\alpha>)\,|+> \;+\; (<-|\alpha>)\,|->$$

but we try to avoid writing two bras or two kets next to each other in this way. A better form is to write the coefficients on the right:

$$\begin{aligned} |\alpha> &= |+><+|\alpha> \;+|-><-|\alpha> \\ |\alpha> &= (|+><+| \;+\; |-><-|)\,|\alpha> \end{aligned}$$

Since $|\alpha>$ is an arbitrary ket, the object in parentheses must be the identity operator,

$$\hat{1} = |+><+| \quad + \quad |-><-|$$

Now let's look at how all this makes sense. The numbers a, b are the components of the vector $|\alpha>$ in our z-basis, so in that basis we may write

$$|\alpha> \;\leftrightarrow\; \begin{pmatrix} a \\ b \end{pmatrix}$$

This is comparable to writing

$$\mathbf{v} \leftrightarrow \begin{pmatrix} v^1 \\ v^2 \\ v^3 \end{pmatrix}$$

for an ordinary 3-vector. Dotting with our Cartesian basis gives the individual components,

$$\begin{aligned} \hat{\mathbf{i}} \cdot \mathbf{v} &= v^1 \\ \hat{\mathbf{j}} \cdot \mathbf{v} &= v^2 \\ \hat{\mathbf{k}} \cdot \mathbf{v} &= v^3 \end{aligned}$$

in perfect analogy to

$$\begin{aligned} <+|\alpha> &= a \\ <-|\alpha> &= b \end{aligned}$$

If we let $\hat{\mathbf{e}}_i = \left(\hat{\mathbf{i}}, \hat{\mathbf{j}}, \hat{\mathbf{k}}\right)$ for $i = 1, 2, 3$ then we can write

$$\hat{\mathbf{e}}_i \cdot \mathbf{v} = v_i$$

where the numbers on the right are the components of the vector $\mathbf{v}$ in the basis $\hat{\mathbf{e}}_i$. Similarly, if we let $< a'| =< \pm|$ as a' takes values $1, 2$, (or $\pm$ if we like) then the components a, b of our ket $|\alpha>$ may be written as

$$< a'|\alpha >$$

Thus, the numbers $< a'|\alpha >$ are the components of the formal vector $|\alpha>$.

4 Operators

We have seen one operator already – the identity,

$$\hat{1} = |+><+| \quad + \quad |-><-|$$

More generally, just as we take a bra-ket combination as the inner product of two vectors, we may take these ket-bra combinations as matrices. This works just like the outer product of a pair of vectors in our ordinary notation,

$$\begin{aligned}\left[\mathbf{u}\otimes\mathbf{v}\right]_{ij} &= u_i v_j \\ &= \begin{pmatrix} u_1v_1 & u_1v_2 & u_1v_3 \\ u_2v_1 & u_2v_2 & u_2v_3 \\ u_3v_1 & u_3v_2 & u_3v_3 \end{pmatrix}\end{aligned}$$

The orthonormality relation shows that in the $\pm$ basis,

$$\begin{aligned}< a'|+> &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ < a'|-> &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}\end{aligned}$$

Now look at the outer products:

$$\begin{aligned}&|+><+| \\ &|-><-|\end{aligned}$$

These are formal outer products, like $\mathbf{uv}$. Corresponding to components u_iv_j we have the matrices,

$$\begin{aligned}< a'|+><+|a''> &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\end{aligned}$$

where we get all four components as a' and a'' range over $\pm$.

Similarly, the outer product $|-><-|$ has matrix components

$$< a'|+><+|a''> = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

When we add these together, we have the identity.

If we want to write a more general operator, we may take a linear combination of all four possibilities:

$$\begin{aligned}< a'|+><+|a''> &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ < a'|+><-|a''> &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ < a'|+><+|a''> &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ < a'|+><+|a''> &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}$$

A general linear combination gives the most general possible 2-dimensional linear operator,

$$\hat{M} = a|+><+| + b|+><-| + c|-><+| + d|-><-|$$

This is the basis-free representation which, in the $|\pm>$ basis, has components

$$\left[\hat{M}\right]_{ij} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

4.1 Generalization

These considerations all apply no matter how many eigenstates there are. Suppose we are interested in a system described by a Hamiltonian operator, $\hat{H}$. Because $\hat{H}$ is Hermitian, will have real eigenvalues, and its eigenvectors of $\hat{H}$ may be chosen to form a complete, orthonormal set. Each eigenvector $|a'>$ satisfies

$$\hat{H}|a> \quad = \quad a|a>$$

where we label the eigenvector $|a>$ with the corresponding eigenvalue. Suppose the full set of eigenvalues is $\{a_1, a_2, \ldots, a_n\}$. Then we have one eigenvector for each eigenvalue, and they span the full space of states. If we wish to index the full set of eigenvectors or eigenvalues, we will use primes, $a', a'', a''' \ldots$ just the way we use indices $i, j, k = 1, 2, 3$ for the components of 3-vectors. Each primed index ranges over the full set of eigenvalues, $a' \in \{a_1, a_2, \ldots, a_n\}$. Thus,

$$\hat{H}|a'> \quad = \quad a'|a'>$$

refers to all n eigenvalue equations as a' ranges from a_1 to a_n.

Since the set of n vectors $\{|a'>: a' = a_1, \ldots, a_n\}$ is orthonormal, we write

$$< a'|a'' > \quad = \quad \delta_{a'a''}$$

This expresses n^2 different inner products, since both a' and a'' range over all of the eigenvalues. Any state of the system may be written as a linear combination of the eigenvectors:

$$|\psi> \quad = \quad \sum_{a'=a_1}^{a_n} \alpha_{a'}|a'>$$

We can find the components of $|\psi>$ by projecting in the direction of each eigenvector,

$$\begin{aligned} < a''|\psi > \quad &= \quad < a''| \left(\sum_{a'=a_1}^{a_n} \alpha_{a'}|a'> \right) \\ &= \quad \sum_{a'=a_1}^{a_n} \alpha_{a'} < a''|a'> \\ &= \quad \sum_{a'=a_1}^{a_n} \alpha_{a'} \delta_{a'a''} \\ &= \quad \alpha_{a''} \end{aligned}$$

We can derive this result in reverse. Given any state, $|\psi>$, we may multiply by the n-dimensional identity operator. But the identity operator may be written as

$$\hat{1} = \sum_{a'=a_1}^{a_n} |a'>< a'|$$

This is evident if we remember that any one eigenvector, $|a_k>$, has components

$$< a'|a_k > \quad = \quad \delta_{a'k}$$

If we write this as a column vector, it is just

$$\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

where the 1 occurs in the k^{th} position. Then,

$$
\begin{aligned}
|a_k><a_k| &= \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{pmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & & & & & & \\ \vdots & & & & & & \\ 0 & & & & & & \\ 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 0 & & & & & & \\ \vdots & & & & & & \\ 0 & & & & & & \end{pmatrix}
\end{aligned}
$$

where the single non-zero entry is the 1 in the k^{th} row and the k^{th} column. When we sum such outer products over all values $a' = a_1, \dots, a_n$ we build up the identity matrix.

Now, let this form of the identity matrix act on a general state, $|\psi>$,

$$
\begin{aligned}
|\psi> &= \hat{1}|\psi> \\
&= \sum_{a'=a_1}^{a_n} |a'><a'|\psi> \\
&= \sum_{a'=a_1}^{a_n} \alpha_{a'}|a'>
\end{aligned}
$$

and we recover the expansion of the state in the given basis.

The basis states do not have to be eigenkets of the Hamiltonian operator. Since the eigenstates of any Hermitian operator form a complete, orthonormal set, we may use any such kets as our basis.

One question remains. Why do we use the index a' to label kets as $|a'>$, instead of just using $|k>$ to label the k^{th} eigenstate? The answer is that we want our notation to include states as general as the wave function, where the number of basis states may be uncountable. This means that instead of writing an arbitrary state $|\psi>$ as a sum over n eigenstates, we must perform an integral,

$$
|\psi> = \int da'|a'><a'|\psi>
$$

In this case, the components of the state together give a function,

$$
<a'|\psi> = \psi(a')
$$

For example, there might be continuum eigenstates of the momentum operator, in which case we write

$$
\begin{aligned}
<p'|\psi> &= \psi(p') \\
|\psi> &= \int dp'|p'><p'|\psi> \\
&= \int dp'\psi(p')|p'>
\end{aligned}
$$

In this case, the normalization requires a Dirac delta function,

$$< p'|p'' > \quad = \quad \delta\left(p' - p''\right)$$

This allows us to find the components,

$$\begin{aligned} |\psi > &= \int dp' \psi\left(p'\right) |p' > \\ < p''|\psi > &= \int dp' \psi\left(p'\right) < p''|p' > \\ &= \int dp' \psi\left(p'\right) \delta\left(p'' - p'\right) \\ &= \psi\left(p''\right) \end{aligned}$$

We will work with these representations extensively in later chapters.

5 Quantum mechanics from wave mechanics

Now return to our basic properties of wave mechanics. We would like to generalize each of these in a way that lets us recover wave mechanics. We take the properties one at a time.

5.1 The wave function

We replace the wave function by a vector in Hilbert space, without necessarily specifying a basis,

$$\psi\left(\mathbf{x}\right) \Longrightarrow |\psi\rangle$$

To recover the wave function, we use the identity operator expressed in a *coordinate* basis. Let the kets $|\mathbf{x}\rangle$ be eigenstates of the position operator, $\hat{\mathbf{X}}$, so that

$$\hat{\mathbf{X}} |\mathbf{x}\rangle = \mathbf{x} |\mathbf{x}\rangle$$

Since the eigenvalues are real, the operator is hermitian. In terms of these, the identity operator is the sum over all $\mathbf{x}$ of $|\mathbf{x}\rangle \langle\mathbf{x}|$, i.e., the integral

$$\hat{1} = \int d^3x |\mathbf{x}\rangle \langle\mathbf{x}|$$

Acting on the state $|\psi\rangle$ with the identity operator, we find

$$\begin{aligned} \hat{1} |\psi\rangle &= \int d^3x \left(|\mathbf{x}\rangle \langle\mathbf{x}|\right) |\psi\rangle \\ |\psi\rangle &= \int d^3x |\mathbf{x}\rangle \langle\mathbf{x} \mid \psi\rangle \end{aligned}$$

This is the expansion of the state $|\psi\rangle$ in a coordinate basis. The coefficients in the expansion, the components of $|\psi\rangle$ in terms of basis vectors $|\mathbf{x}\rangle$, are the inner products

$$\langle\mathbf{x} \mid \psi\rangle$$

This object is a complex number for each value of the coordinte $\mathbf{x}$. Naming the function ψ, we identify

$$\psi\left(\mathbf{x}\right) = \langle\mathbf{x} \mid \psi\rangle$$

5.2 Normalization and probability densities

A state is normalized using the inner product,

$$\langle \psi \mid \psi \rangle = 1$$

and this will be true in any basis. In particular, again inserting the coordinate basis identity operator

$$\begin{aligned} 1 &= \langle \psi \mid \psi \rangle \\ &= \langle \psi | \left(\int d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}| \right) |\psi\rangle \\ &= \int d^3x \, \langle \psi \mid \mathbf{x} \rangle \langle \mathbf{x} \mid \psi \rangle \\ &= \int d^3x \psi^* (\mathbf{x}) \psi (\mathbf{x}) \end{aligned}$$

we recover the wave function normalization.

We may find not only the position probability density,

$$P(V) = \int_V d^3x \, \langle \psi \mid \mathbf{x} \rangle \langle \mathbf{x} \mid \psi \rangle = \int_V d^3x \psi^* (\mathbf{x}) \psi (\mathbf{x})$$

but the density in any basis. For example we can find the probability of finding the particle in a volume Φ of momentum space. Let $\varphi(\mathbf{p}) = \langle \mathbf{p} \mid \psi \rangle$. Then,

$$P(\Phi) = \int_\Phi d^3p \, \langle \psi \mid \mathbf{p} \rangle \langle \mathbf{p} \mid \psi \rangle = \int_V d^3x \varphi^* (\mathbf{p}) \varphi (\mathbf{p})$$

5.3 Hermitian operators for dynamical variables

There are various Hermitian linear operators for dynamical variables, also called physical observables, such as position, energy and momentum. These three are given by

$$\begin{aligned} \hat{\mathbf{x}} &= \mathbf{x} \\ \hat{E} &= i\hbar \frac{\partial}{\partial t} \\ \hat{\mathbf{p}} &= -i\hbar \boldsymbol{\nabla} \end{aligned}$$

These may be seen as coordinate basis representations of Hilbert space operators. Thus, if we define the Hermitian position operator by

$$\hat{\mathbf{X}} |\mathbf{x}\rangle = \mathbf{x} |\mathbf{x}\rangle$$

it's representation a coordinate basis is,

$$\begin{aligned} \langle \mathbf{x}' | \hat{\mathbf{X}} |\mathbf{x}\rangle &= \mathbf{x} \langle \mathbf{x}' \mid \mathbf{x} \rangle \\ &= \mathbf{x} \delta^3 (\mathbf{x}' - \mathbf{x}) \end{aligned}$$

that is, multiplying by $\mathbf{x}$.

Thus, for example, we may find the the potential term of the Schrödinger equation, $\hat{V}(\mathbf{x}) \equiv V\left(\hat{\mathbf{X}}\right)$, in the coordinate basis. Restricting to one dimension to keep the Taylor series simple, its matrix components are

$$\begin{aligned} \langle \mathbf{x}' | V\left(\hat{X}\right) |\mathbf{x}\rangle &= \langle x' | \sum_{n=0}^{\infty} \frac{1}{n!} V^{(n)}(0) \hat{X}^n |x\rangle \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} V^{(n)}(0) \langle x' | \hat{X}^n |x\rangle \end{aligned}$$

We evaluate the expectation value one operator at a time, $\langle x'|\,\hat{X}^n\,|x\rangle = \langle x'|\,\hat{X}^{n-1}x\,|x\rangle = \cdots = \langle x'|\,x^n\,|x\rangle = x^n\delta\left(x'-x\right)$, giving

$$\begin{aligned}\langle \mathbf{x}'|\,V\left(\hat{X}\right)|\mathbf{x}\rangle &= \sum_{n=0}^{\infty}\frac{1}{n!}V^{(n)}\left(0\right)x^n\delta\left(x'-x\right)\\ &= V\left(x\right)\delta\left(x'-x\right)\end{aligned}$$

In this basis, therefore, the potential or any function of position only, becomes a diagonal operator.

The story is different in the momentum basis. Letting $\hat{\mathbf{X}}$ act on a momentum basis ket,

$$\begin{aligned}\hat{\mathbf{X}}\,|\mathbf{p}\rangle &= \int\limits_{\Phi} d^3x'\hat{\mathbf{X}}\,|\mathbf{x}'\rangle\,\langle\mathbf{x}'\mid\mathbf{p}\rangle\\ &= \frac{1}{\sqrt{2\pi}}\int\limits_{\Phi} d^3x'\mathbf{x}'e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}'}\,|\mathbf{x}'\rangle\\ &= \frac{1}{\sqrt{2\pi}}\int\limits_{\Phi} d^3x'\left(i\hbar\boldsymbol{\nabla}_{\mathbf{p}}\right)e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}'}\,|\mathbf{x}'\rangle\end{aligned}$$

$$\begin{aligned}\langle\mathbf{p}'|\,\hat{\mathbf{X}}\,|\mathbf{p}\rangle &= \left(i\hbar\boldsymbol{\nabla}_{\mathbf{p}}\right)\left[\frac{1}{\sqrt{2\pi}}\int\limits_{\Phi} d^3x'e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}'}\,\langle\mathbf{p}'\mid\mathbf{x}'\rangle\right]\\ &= \left(i\hbar\boldsymbol{\nabla}_{\mathbf{p}}\right)\left[\frac{1}{2\pi}\int\limits_{\Phi} d^3x'e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}'}e^{\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'}\right]\\ &= \left(i\hbar\boldsymbol{\nabla}_{\mathbf{p}}\right)\delta^3\left(\mathbf{p}-\mathbf{p}'\right)\end{aligned}$$

This time, the potential will become a derivative operator, $\langle\mathbf{p}'|\,V\left(\hat{X}\right)|\mathbf{p}\rangle = V\left(i\hbar\boldsymbol{\nabla}_{\mathbf{p}}\right)\delta^3\left(\mathbf{p}-\mathbf{p}'\right)$. As always, the derivative of a delta function is handled by integration by parts when the expression is integrated.

5.4 Replacement of the state after measurement

Measurement of a dynamical variable always yields an eigenvalue of the corresponding linear operator, and changes the state to the corresponding eigenvector. It is modeled by allowing the operator corresponding to the dynamical variable act on the wave function. In wave mechanics this statement says that a state ψ, expanded in eigenstates $\varphi_a\left(\mathbf{x}\right)$ of an Hermitian operator $\hat{\mathcal{A}}$,

$$\psi = \int A\left(a\right)\varphi_a\left(\mathbf{x}\right)da$$

will be replaced after measurement. If we measure the value a_0 for the observable $\hat{\mathcal{A}}$, then the state $\psi\left(\mathbf{x}\right)$ is replaced by the single corresponding eigenstate,

$$\psi'\left(\mathbf{x}\right) = A\left(a_0\right)\varphi_{a_0}\left(\mathbf{x}\right)$$

In Dirac notation, the state is a vector and the expansion is

$$|\psi\rangle = \int daA\left(a\right)|a\rangle$$

where $\hat{\mathcal{A}}\left|a\right\rangle = a\left|a\right\rangle$. In a coordinate basis, this becomes

$$\begin{aligned}\left\langle \mathbf{x}\mid\psi\right\rangle &= \int daA\left(a\right)\left\langle \mathbf{x}\mid a\right\rangle \\ \psi\left(\mathbf{x}\right) &= \int daA\left(a\right)\varphi_{a}\left(\mathbf{x}\right)\end{aligned}$$

and we recover the wave mechanics form. The replacement after measurement, is simply

$$\left|\psi'\right\rangle = A\left(a_{0}\right)\left|a_{0}\right\rangle$$

5.5 Evolution of the state between measurements

Between measurements, the state evolves according to the Schrödinger equation,

$$-\frac{\hbar}{2m}\nabla^{2}\psi\left(\mathbf{x}\right)+V\left(\mathbf{x}\right)\psi=E\psi\left(\mathbf{x}\right)$$

and we expect this to be represented by the eigenvalue problem,

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

We are obliged to find the form of the Hamiltonian operator such that in a coordinate basis,

$$\left\langle \mathbf{x}\right|\hat{H}\left|\psi\right\rangle = E\left\langle \mathbf{x}\mid\psi\right\rangle$$

we recover the Schrödinger wave equation. The result is immediate if we write the Hamiltonian properly as a function of position and momentum,

$$H\left(\mathbf{x},\mathbf{p}\right)\Rightarrow\hat{H}=H\left(\hat{\mathbf{X}},\hat{\mathbf{P}}\right)$$

We simply replace $\mathbf{x}$ and $\mathbf{p}$ by the corresponding operators. Checking that we recover the Schrödinger equation,

$$\begin{aligned}\left\langle \mathbf{x}'\right|\hat{H}\left|\mathbf{x}\right\rangle &= \left\langle \mathbf{x}'\right|H\left(\hat{\mathbf{X}},\hat{\mathbf{P}}\right)\left|\mathbf{x}\right\rangle \\ &= \left\langle \mathbf{x}'\right|\frac{1}{2m}\hat{\mathbf{P}}^{2}+V\left(\hat{\mathbf{X}}\right)\left|\mathbf{x}\right\rangle \\ &= \frac{1}{2m}\left\langle \mathbf{x}'\right|\hat{\mathbf{P}}^{2}\left|\mathbf{x}\right\rangle +\left\langle \mathbf{x}'\right|V\left(\hat{\mathbf{X}}\right)\left|\mathbf{x}\right\rangle \\ &= \frac{1}{2m}\left\langle \mathbf{x}'\right|\hat{\mathbf{P}}^{2}\left|\mathbf{x}\right\rangle +V\left(\mathbf{x}'\right)\delta^{3}\left(\mathbf{x}'-\mathbf{x}\right)\end{aligned}$$

For the momentum operator, we introduce the momentum basis identity,

$$\begin{aligned}\left\langle \mathbf{x}'\right|\hat{\mathbf{P}}^{2}\left|\mathbf{x}\right\rangle &= \int d^{3}p\left\langle \mathbf{x}'\right|\hat{\mathbf{P}}^{2}\left|\mathbf{p}'\right\rangle \left\langle \mathbf{p}\right|\left|\mathbf{x}\right\rangle \\ &= \int d^{3}p\left\langle \mathbf{x}'\right|\mathbf{p}'^{2}\left|\mathbf{p}'\right\rangle \left\langle \mathbf{p}\mid\mathbf{x}\right\rangle \\ &= \int d^{3}p\mathbf{p}'^{2}\left\langle \mathbf{x}'\mid\mathbf{p}'\right\rangle \left\langle \mathbf{p}\mid\mathbf{x}\right\rangle \\ &= \frac{1}{2\pi}\int d^{3}p\mathbf{p}'^{2}e^{-\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}} \\ &= \frac{1}{2\pi}\int d^{3}p\left(i\hbar\nabla_{x'}\right)^{2}e^{-\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}} \\ &= \left(i\hbar\nabla_{x'}\right)^{2}\delta^{3}\left(\mathbf{x}'-\mathbf{x}\right)\end{aligned}$$

and finally

$$\begin{aligned}\hat{H} &= \frac{1}{2m}\left(i\hbar\nabla_{x'}\right)^2\delta^3\left(\mathbf{x}'-\mathbf{x}\right)+V\left(\mathbf{x}'\right)\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\\ &= \left(-\frac{\hbar^2}{2m}\nabla_{x'}^2+V\left(\mathbf{x}'\right)\right)\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\end{aligned}$$

Integrating by parts twice returns us to the Schrödinger equation

$$\begin{aligned}\hat{H}\left|\psi\right\rangle &= E\left|\psi\right\rangle\\ \int d^3x'\left\langle\mathbf{x}\right|\hat{H}\left|\mathbf{x}'\right\rangle\left\langle\mathbf{x}'\mid\psi\right\rangle &= E\left\langle\mathbf{x}\mid\psi\right\rangle\\ \int d^3x'\left(-\frac{\hbar^2}{2m}\nabla_{x'}^2+V\left(\mathbf{x}'\right)\right)\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\psi\left(\mathbf{x}'\right) &= E\psi\left(\mathbf{x}\right)\\ \int d^3x'\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\left(-\frac{\hbar^2}{2m}\nabla_{x'}^2+V\left(\mathbf{x}'\right)\right)\psi\left(\mathbf{x}'\right) &= E\psi\left(\mathbf{x}\right)\\ \left(-\frac{\hbar^2}{2m}\nabla_x^2+V\left(\mathbf{x}\right)\right)\psi\left(\mathbf{x}\right) &= E\psi\left(\mathbf{x}\right)\end{aligned}$$

5.6 Spin states

We have seen in detail how to represent spin states and operators.