Chapter 6. The Coordinate Representation

§ 1 *Introduction.* A pure state $|x\rangle$ of the position operator is a state in which we know for certain that the coordinate of the particle is x. For now I assume that the system is one-dimensional, to keep the notation as simple as possible. Because position is an observable, its pure states (which are the eigenstates of the position operator) form a complete basis set that can be used to represent abstract kets. The representation generated by using pure position kets plays a central role in quantum mechanics because it connects the abstract kets of Dirac theory to the Schrödinger wave function. Schrödinger's formulation of quantum mechanics is Dirac's theory in coordinate representation.

§ **2** *The spectrum of the position operator is continuous.* We have postulated that the position operator has a continuous spectrum, which means that there is no natural law that prevents the position from changing by an infinitesimal amount.

One should be careful to distinguish between what is impossible and what is improbable. To explain the distinction I use the harmonic oscillator as an illustration. Its energy is discrete, which means that it is *impossible* for the energy to take a value different from $\hbar\omega(n+1/2)$, where n can be 0, 1, 2, ... I do not mean unlikely: I mean impossible. Contrast this with the position x of an oscillator that vibrates around the point x_0. The probability that an oscillator in the ground state is located at x is proportional to the Gaussian function

$$\exp[\beta(x-x_0)^2]$$

where β is a real number. This equation tells us that it is very improbable that the position x of the oscillator is very far from x_0. x can take any value; it is just that the forces in the system (the spring, in the case of the oscillator) make it unlikely for x to differ too much from x_0.

§ **3** *The pure states of the position.* In Chapter 2 I introduced a special normalization for the pure states of the continuous spectrum, by analogy with the discrete spectrum. If $|x\rangle$ and $|y\rangle$ are two pure states of the position then

$$\langle y \,|\, x\rangle = \delta(y-x) \tag{1}$$

The Dirac δ is defined to have the properties

$$\int \mathrm{d}x\, \delta(y-x)\, f(x) = f(y) \tag{2}$$

for any “well behaved” function $f(y)$. In addition we require that

$$\delta(x) = 0 \quad \text{if } x \neq 0 \tag{3}$$

§ 4 *Can we make a pure state of position in the laboratory?* Quantum mechanics gives us rules for working with symbols such as $|x\rangle$. Before we use them let’s examine whether it is possible to perform experiments in which a particle is forced to have the state $|\,x\rangle$. This is not a “practical” question because it is unlikely that any one will attempt such experiments. However, thinking about it will improve our ability to connect the formalism of quantum mechanics to reality.

There are reasons to believe that the answer is not simple. First, according to the uncertainty principle, if the position is known precisely then all momenta are equally probable (we will give a proof of this statement when we discuss the momentum representation). It is difficult to imagine how one creates a state in which we have absolutely no information about momentum (any value is as probable as any other). Any practical device used to localize a particle would put some limits on the values of its momentum and therefore prevent us from creating a pure state $|x\rangle$.

Eq. 1 should also cause some anxiety. To see why, let us change the notation so that $|\psi\rangle \equiv |x\rangle$. We can rewrite Eq. 1 as

$$\langle y \,|\, \psi\rangle \equiv \delta(y - x) \tag{4}$$

The symbol in the left-hand side of this equation is the Schrödinger wave function of the ket $|\psi\rangle \equiv |x\rangle$. This “wave function” is not a function (the delta function is not a function) and it is highly singular. This, again, tells us that there is something unusual about the state $|x\rangle$.

Whenever the mathematics is bewildering we need to turn to physics. We can localize a particle by performing a "thought experiment". We can put the particle in a box whose walls are impenetrable (the potential energy for the particle outside the box is infinity and it is zero inside). Nobody knows how to make such a box but let's ignore that and assume that we have a box like that. You can think of the box as a device measuring the location of the particle: the smaller the box size, the more accurate is our knowledge of the position. In the limit when the box size L goes to zero, we know exactly the position of the particle.

However, when L is made smaller the energy of the particle (which is $\frac{\hbar^2}{2m}(\frac{\pi k}{L})^2$) increases. This means that whatever device is used to make L smaller will have to provide work. A perfect localization would require an infinite amount of energy. This behavior is general in quantum mechanics: localizing a particle increases its energy.

We can do another thought experiment in which we use a harmonic oscillator and localize the particle by increasing the force constant k of the spring, to make the spring stronger and stronger. As k increases, the amplitude of the oscillation becomes smaller and smaller and the particle is more and more localized. Since the frequency of the oscillator is proportional to the square root of k, as k goes to infinity the frequency ω goes to infinity and so does the energy. Again, to localize the particle we need to provide work; perfect localization requires an infinite amount of work.

While it is unlikely that one creates pure states of position in the laboratory, the state

$$|\psi\rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\ f(x)|x\rangle \tag{5}$$

is achievable. The function $f(x)$ can be a bell-shape function (such as a Gaussian). The probability that a particle in this state is located at y is

$$|\langle y \,|\, \psi\rangle|^2 = \Big| \int_{-\infty}^{+\infty} \mathrm{d}x \; f(x)\,\delta(y-x) \Big|^2 \equiv |f(y)|^2 \tag{6}$$

The function f controls where the particle is located.

§ 5 *Completeness relation.* Of utmost importance to what follows is that the pure states of position must satisfy the completeness relation

$$\hat{I} = \int_{-\infty}^{+\infty} \mathrm{d}x \,|x\rangle\,\langle x| \tag{7}$$

This must be so because position is an observable. The completeness relation allows us to express any ket $|\psi\rangle$ in the *coordinate representation*:

$$|\psi\rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x \; |x\rangle\,\langle x \,|\, \psi\rangle \tag{8}$$

The quantity $\langle x \,|\, \psi\rangle$ is the Schrödinger wave function $\psi(x)$ of the system in state $|\psi\rangle$. The probability $P_\psi(x)\,\mathrm{d}x$ that a system in state $|\psi\rangle$ is located in the space interval $\mathrm{d}x$ centered around the position x is

$$P_\psi(x)\,\mathrm{d}x \equiv |\langle x \,|\, \psi\rangle|^2\,\mathrm{d}x \equiv \psi(x)^*\psi(x)\,\mathrm{d}x \tag{9}$$

§ 6 *Generalization of the coordinate representation to three dimensions and more than one particle.* For a particle in three dimensions, we denote by $|x, y, z\rangle$ or $|\vec{r}\rangle$ a pure state in which the particle is at position $\vec{r} \equiv \{x, y, z\}$ with x, y, and z being the components of the position vector $\vec{r}$ in a Cartesian coordinate system.

If we perform an experiment that places the system in a state $|\psi\rangle$ then

$$P_\psi(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \equiv |\langle x, y, z \,|\, \psi\rangle|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

is the probability that a measurement of the position will find the particle in the volume $\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ centered around $\vec{r} = \{x, y, z\}$.

As we have seen in Chapter 2, the completeness relation follows from this formula for the probability and if you follow the procedure used there you can show that

$$\int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x, y, z\rangle\,\langle x, y, z| = \hat{I} \tag{10}$$

and that we can write

$$|\psi\rangle = \hat{I}|\psi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x, y, z\rangle\,\langle x, y, z\,|\,\psi\rangle \tag{11}$$

We have also seen in Chapter 2 that

$$\langle x, y, z\,|\,\psi\rangle \equiv \psi(x, y, z)$$

is the Schrödinger wave function, generalized in this case for a particle located in a three-dimensional space.

Eq. 11 leads to

$$\langle x', y', z'\,|\,\psi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\langle x', y', z'\,|\,x, y, z\rangle\,\langle x, y, z\,|\,\psi\rangle, \tag{12}$$

which is possible only if

$$\langle x', y', z'\,|\,x, y, z\rangle = \delta(x - x')\,\delta(y - y')\,\delta(z - z') \equiv \delta(\vec{r} - \vec{r}') \tag{13}$$

This is an "obvious" generalization of Dirac's delta function to three dimensions.

For n particles, all in a three-dimensional space, a pure position state is

$$|\vec{r}(1), \vec{r}(2), \ldots, \vec{r}(n)\rangle = |x(1), y(1), z(1), x(2), y(2), z(2), \ldots, x(n), y(n), z(n)\rangle$$

The index i in $\vec{r}(i)$ tells us that this is the position of the i-th particle. Alternative notations are

$$|\vec{r}(1), \vec{r}(2), \ldots, \vec{r}(N)\rangle \tag{14}$$

and

$$|x_1(1), x_2(1), x_3(1), x_1(2), x_2(2), x_3(2), \ldots, x_1(N), x_2(N), x_3(N)\rangle \tag{15}$$

The completeness relation is

$$\hat{I} = \int \mathrm{d}\vec{r}(1) \cdots \mathrm{d}\vec{r}(n)\, |\vec{r}(1), \vec{r}(2), \ldots, \vec{r}(n)\rangle \, \langle \vec{r}(1), \vec{r}(2), \ldots, \vec{r}(n)|$$

with $\mathrm{d}\vec{r}(k) = \mathrm{d}x(k)\,\mathrm{d}y(k)\,\mathrm{d}z(k)$ or $\mathrm{d}x_1(k)\,\mathrm{d}x_2(k)\,\mathrm{d}x_3(k)$, depending on which of the above notations is used.

The normalization is

$$\begin{aligned}
\langle \vec{r}(1), \ldots, \vec{r}(n) \,|\, \vec{r}'(1), \ldots, \vec{r}'(n)\rangle &= \delta(\vec{r}(1) - \vec{r}'(1)) \cdots \delta(\vec{r}(n) - \vec{r}'(n)) \\
&= \delta(x(1) - x'(1))\delta(y(1) - y'(1)) \cdots \delta(z(n) - z'(n)) \\
&= \prod_k \delta(x(k) - x'(k))\, \delta(y(k) - y'(k))\, \delta(z(k) - z'(k))
\end{aligned}$$

If $|\psi\rangle$ is a ket representing the state of an system consisting of N particles, the corresponding Schrödinger wave function is

$$\psi(x(1), y(1), z(1) \ldots, x(N), y(N), z(N)) = \langle x(1), y(1), z(1) \ldots, x(N), y(N), z(N) \,|\, \psi\rangle$$

This is the single most miserable feature of quantum mechanics: the essential quantity of the theory of N interacting particles is a function of $3N$ variables. This makes numerical calculations in quantum mechanics extremely difficult. Computations in any other branch of physics are much, much simpler because the quantities that are calculated are functions of only three coordinates and time.

§ **7** *The coordinate operator.* According to general theory, for each observable A we can construct an operator (see Chapter 4)

$$\hat{A} = \sum_n |a_n\rangle \, a_n \, \langle a_n| + \int_{\alpha \in D} |\alpha\rangle \, \alpha \, \langle \alpha| \, \mathrm{d}\alpha \tag{16}$$

where $\{a_1, a_2, \ldots\}$ and $\alpha \in D$ is the spectrum of A and $|a_n\rangle$ and $|\alpha\rangle$ are the corresponding pure states.

We can apply this to the coordinate since position is an observable. Therefore, in one dimension, we associate with the coordinate an operator $\hat{c}$ defined by

$$\hat{c} = \int_{-\infty}^{+\infty} \mathrm{d}x \, |x\rangle \, x \, \langle x| \tag{17}$$

where $|x\rangle$ is the pure state of position.

We have

$$\begin{array}{ll} \hat{c}|y\rangle & = \int_{-\infty}^{+\infty} \mathrm{d}x \, |x\rangle \, x \, \langle x \mid y\rangle \\ & = \int_{-\infty}^{+\infty} \mathrm{d}x \, |x\rangle \, x \, \delta(y - x) \quad \text{(used Eq. 1)} \\ & = y|y\rangle \qquad\qquad\qquad\qquad \text{(used Eq. 2)} \end{array}$$

In summary,

$$\hat{c}|y\rangle = y|y\rangle \tag{18}$$

This is what we expect: the pure states of position are eigenstates of the coordinate operator and the possible values of the coordinate (its spectrum) are eigenvalues of that operator.

The generalization to three dimensions must be made carefully because the position $\vec{r}$ is a vector. Therefore the operator corresponding to $\vec{r}$ must also be a vector. We write it as

$$\hat{\vec{r}} = \{\hat{x}, \hat{y}, \hat{z}\}$$

where

$$
\begin{aligned}
\hat{x} &\equiv \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x,y,z\rangle\, x\,\langle x,y,z| \\
\hat{y} &\equiv \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x,y,z\rangle\, y\,\langle x,y,z| \\
\hat{z} &\equiv \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x,y,z\rangle\, z\,\langle x,y,z|
\end{aligned}
$$

are the components of the vector operator $\hat{\vec{r}}$. We have, for example,

$$
\begin{aligned}
\hat{x}|x',y',z'\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x,y,z\rangle\, x\,\langle x,y,z\,|\,x',y',z'\rangle \\
&= \int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|x,y,z\rangle\, x\,\delta(x-x')\delta(y-y')\delta(z-z') \quad \text{(used Eq. 13)} \\
&= x'|x',y',z'\rangle
\end{aligned}
$$

Similar results are obtained for $\hat{y}|x',y',z'\rangle$ and $\hat{z}|x',y',z'\rangle$; they are the generalization to three dimensions of Eq. 18.

You should be able to generalize this to the case of several particles in three-dimensional space.

§ 8 *Operators that are functions of coordinate.* The general theory told us that if an operator $\hat{A}$ is defined by

$$
\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\,\langle a_n| + \int_{\alpha\in D} \mathrm{d}\alpha\,|\alpha\rangle\,\alpha\,\langle\alpha| \tag{19}
$$

then a function $f(\hat{A})$ is defined by

$$
f(\hat{A}) = \sum_{n=1}^{\infty} |a_n\rangle\, f(a_n)\,\langle a_n| + \int_{\alpha\in D} \mathrm{d}\alpha\,|\alpha\rangle\, f(\alpha)\,\langle\alpha| \tag{20}
$$

Apply this to the position operator in a one-dimensional system. Since

$$
\hat{c} = \int_{-\infty}^{+\infty} |x\rangle\, x\,\langle x|\,\mathrm{d}x \tag{21}
$$

the operator corresponding to a function $f(x)$ is

$$f(\hat{c}) \equiv \int_{-\infty}^{+\infty} |x\rangle\, f(x)\, \langle x|\, \mathrm{d}x \tag{22}$$

which gives

$$\begin{aligned} f(\hat{c})|y\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}x\, |x\rangle\, f(x)\, \langle x \,|\, y\rangle \\ &= \int_{-\infty}^{+\infty} \mathrm{d}x\, |x\rangle\, f(x)\, \delta(x-y) = f(y)|y\rangle \end{aligned} \tag{23}$$

This result is very important because when we define the total energy operator (the Hamiltonian) we need to define an operator for the potential energy. A natural recipe is to use the classical potential energy $V(x)$ and construct the corresponding potential energy operator

$$V(\hat{c}) \equiv \int_{-\infty}^{+\infty} |x\rangle\, V(x)\, \langle x|\, \mathrm{d}x \tag{24}$$

Exercise 1 Write an expression for the potential energy of a harmonic oscillator.

It is easy to show that

$$V(\hat{c})|y\rangle = \int_{-\infty}^{+\infty} |x\rangle\, V(x)\, \langle x|y\rangle\, \mathrm{d}x \equiv \int_{-\infty}^{+\infty} |x\rangle\, V(x)\, \delta(x-y)\, \mathrm{d}x \equiv V(y)|y\rangle \tag{25}$$

I remind you that coordinate representation is used very often to calculate various scalar products needed in quantum mechanical calculations, such as

$$\langle \psi \,|\, \phi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x \langle \psi \,|\, x\rangle\langle x \,|\, \phi\rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\ \psi(x)^* \phi(x) \tag{26}$$

An useful example of such calculation is

$$\begin{aligned}\langle y \,|\, V(\hat{c}) \,|\, \psi\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}x \, \langle y \,|\, x\rangle \, V(x) \, \langle x \,|\, \psi\rangle \\ &= \int_{-\infty}^{+\infty} \mathrm{d}x \, \delta(y-x) \, V(x) \, \langle x \,|\, \psi\rangle = V(y)\psi(y)\end{aligned}$$

Remember that

$$\langle y \,|\, V(\hat{c}) \,|\, \psi\rangle = V(y)\langle y \,|\, \psi\rangle = V(y)\psi(y) \tag{27}$$

Since $\langle y \,|\, \psi\rangle$ is the Schrödinger wave function $\psi(y)$, the right-hand side of Eq. 27 is the term in the Schrödinger equation corresponding to the classical potential energy $V(y)$.

We can generalize this easily to n particles each moving in three dimensions,

$$V(\hat{\vec{r}}(1), \ldots, \hat{\vec{r}}(n)) \,|\, \vec{q}(1), \ldots, \vec{q}(n)\rangle = V(\vec{q}(1), \ldots, \vec{q}(n)) \,|\, \vec{q}(1), \ldots, \vec{q}(n)\rangle$$

Note that in the right-hand side of this expression V has the same arguments as the ket.

We must keep in mind that $|x\rangle$ is a state in which the particle is located at x. If the coordinate operator is denoted by $\hat{c}$ then $\hat{c}|x\rangle = x|x\rangle$. The x multiplying $|x\rangle$ is the *eigenvalue* of the operator $\hat{c}$. It is a number that will be obtained if we measure the position when the system is in the state $|x\rangle$. Similarly,

$$\hat{V}(\hat{c})|x\rangle = V(x)|x\rangle$$

The variable x in $V(x)$ is the position of the particle when the system is in the pure state $|x\rangle$. The variable $\hat{c}$ in $\hat{V}(\hat{c})$ is the position operator. $V(x)$ is the value obtained if we measure the potential energy when the particle is in the state $|x\rangle$. $V(x)$ is a function of position whose values are real numbers; $V(\hat{c})$ is an operator.

§ 9 *The central role of the Cartesian system of coordinates.* Have you noticed that throughout this chapter we used Cartesian coordinates? What about problems that have spherical symmetry (e.g. hydrogen atom) or cylindrical symmetry (e.g. H_2^+ ion)? Should we use spherical or cylindrical coordinates? By all means, but the question is at what point in the theoretical analysis do we begin to use them. It is possible to formulate the theory so that it is applicable to any coordinate system. However, the formulation is tedious and uses extensive notation, and it needs to be done carefully. Here is a simpler procedure: write the starting equations in Cartesian coordinates and *after you have done that, convert the equation to the coordinate system that seems more appropriate* (e.g. spherical or cylindrical). Many books[1] give you the information you need for doing that: what the variables are (e.g. a radius, the polar angle, and the azimuthal angle for spherical coordinates), their connection to the Cartesian coordinates, and the formulae for various differential operators such as the Laplacean or the gradient.

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[1] Two classics are Philip M. Morse and Herman Feshbach, *Methods of Theoretical Physics*, New York, McGraw-Hill, 1953; and Henry Margenau and George Moseley Murphy, *The Mathematics of Physics and Chemistry*, Princeton, Van Nostrand, 1956-64. An excellent recent book is George B. Arfken and Hans J. Weber, *Mathematical Methods for Physicists*, Burlington MA, Elsevier Academic Press, 2005.