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The Vector Space Interpretation of Quantum-Mechanical Systems

A Different "Representations" of the State of a Quantum-Mechanical System

So far, we have specified the state of a quantum-mechanical system by the wave function, $\Psi(\vec{r}, t)$, i.e., by specifying the value of the scalar function, Ψ, for all values of x, y, z, at a particular time, t. Ψ could also be specified, however, at a particular time by the infinite set of numbers, $c_n(t)$, in the expansion of $\Psi(\vec{r}, t)$ in the compleete set of energy eigenfunctions of the system,

$$c_n e^{-\frac{i}{\hbar}E_n t} =< \psi_n, \Psi(\vec{r}, t) > \equiv c_n(t), \tag{1}$$

with

$$c_n =< \psi_n, \Psi(\vec{r}, t = 0) > = \int d\vec{r}\psi_n^*(\vec{r})\Psi(\vec{r}, t = 0). \tag{2}$$

Alternatively, Ψ could just as well be specified by another set of numbers, a set of Fourier coefficients of some other (complete) set of generalized Fourier functions. For example, we might use the eigenfunctions of some other Hamiltonian, $\overline{H}$, not the Hamiltonian of *our* system, or possibly $\overline{H}$ could be some other Hermitian operator, not a Hamiltonian. Let us assume, in particular, $\overline{H}$ has both a discrete and a continuous spectrum, where the discrete spectrum is numbered by an index, $i = 1, 2, \ldots, n$, perhaps a finite number or perhaps an infinite number, whereas the continuous eigenvalue spectrum is parameterized by a continuous variable, α, such that

$$\overline{H}u_i(\vec{r}) = E_i u_i(\vec{r}) \tag{3}$$

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$$\overline{H} w_\alpha(\vec{r}) = E(\alpha) w_\alpha(\vec{r}), \tag{4}$$

where the eigenfunctions form an orthonormal set, with

$$< u_i, u_j >= \delta_{ij}, \qquad < u_i, w_\alpha >= 0, \qquad < w_\alpha, w_{\alpha'} >= \delta(\alpha - \alpha'). \tag{5}$$

The eigenfunctions must of course also form a complete set, where the completeness relation is now

$$\sum_i u_i^*(\vec{r}\,') u_i(\vec{r}) + \int d\alpha\, w_\alpha^*(\vec{r}\,') w_\alpha(\vec{r}) = \delta(\vec{r}\,' - \vec{r}). \tag{6}$$

Now, Ψ can be expanded in terms of this complete set via

$$\Psi(\vec{r}, t) = \sum_i c_i u_i(\vec{r}) + \int d\alpha\, c(\alpha) w_\alpha(\vec{r}), \tag{7}$$

where the c_i and $c(\alpha)$ are given by

$$c_i =< u_i, \Psi >= \int d\vec{r}\,' u_i^*(\vec{r}\,') \Psi(\vec{r}\,', t), \tag{8}$$

$$c(\alpha) =< w_\alpha, \Psi >= \int d\vec{r}\,' w_\alpha^*(\vec{r}\,') \Psi(\vec{r}\,', t). \tag{9}$$

The c_i and $c(\alpha)$ are now implicitly time dependent. These c_i and $c(\alpha)$ now give us still another alternative for the description of our quantum-mechanical system.

So far, we have used Fourier expansions in a set of orthonormal functions that themselves were square-integrable functions; i.e., they were themselves part of our Hilbert space. The basis functions in the Fourier expansions, however, need not themselves be square-integrable. In fact, our original expansion in terms of ordinary Fourier plane-wave functions was of this type. The plane-wave functions (in the general notation of this chapter) are

$$u_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r})}. \tag{10}$$

These functions are eigenfunctions simultaneously of the three operators $(p_x)_{\text{op.}}$, $(p_y)_{\text{op.}}$, $(p_z)_{\text{op.}}$, with eigenvalues p_x, p_y, p_z, with, e.g.,

$$\frac{\hbar}{i}\frac{\partial}{\partial x} u_{\vec{p}}(\vec{r}) = p_x u_{\vec{p}}(\vec{r}). \tag{11}$$

Because the spectrum of possible $\vec{p}$ is continuous, the orthogonality is expressed in terms of a Dirac delta function in place of a Kronecker delta

$$< u_{\vec{p}\,'}, u_{\vec{p}} >= \delta(\vec{p}\,' - \vec{p}), \tag{12}$$

and the completeness relation is given by

$$\int d\vec{p}\, u_{\vec{p}}^*(\vec{r}\,') u_{\vec{p}}(\vec{r}) = \delta(\vec{r}\,' - \vec{r}). \tag{13}$$

The Fourier expansion of Ψ is the standard Fourier one, with expansion coefficients, $\phi(\vec{p}, t)$, now the standard Fourier transform

$$\Psi(\vec{r}, t) = \int d\vec{p}\, \phi(\vec{p}, t) u_{\vec{p}}(\vec{r}), \tag{14}$$

with

$$\phi(\vec{p}, t) = < u_{\vec{p}}, \Psi > . \tag{15}$$

The $\phi(\vec{p}, t)$ now give us another alternative way of specifying the state of our quantum-mechanical system.

Finally, we could even use a basis of Dirac delta functions for the generalized Fourier expansion of our Ψ, where these can be written, in analogy with the $u_{\vec{p}}$, or the ψ_n, as

$$u_{\vec{r}_0}(\vec{r}) = \delta(\vec{r} - \vec{r}_0), \tag{16}$$

where these u's are simultaneously the eigenfunctions of the three operators x, y, z; with eigenvalues x_0, y_0, z_0. For example,

$$x u_{\vec{r}_0}(\vec{r}) = x\delta(\vec{r} - \vec{r}_0) = x_0 \delta(\vec{r} - \vec{r}_0), \tag{17}$$

where we have used the delta function relation

$$f(x)\delta(x) = f(0)\delta(x). \tag{18}$$

The orthogonality of the u's is now given by the delta function relation

$$\int d\vec{r} u^*_{\vec{r}_0}(\vec{r}) u_{\vec{r}_0'}(\vec{r}) = \int d\vec{r}\delta(\vec{r} - \vec{r}_0)\delta(\vec{r} - \vec{r}_0') = \delta(\vec{r}_0 - \vec{r}_0'). \tag{19}$$

The completeness relation is now given by the integral

$$\int d\vec{r}_0 u^*_{\vec{r}_0}(\vec{r}\,') u_{\vec{r}_0}(\vec{r}) = \int d\vec{r}_0 \delta(\vec{r}_0 - \vec{r}\,')\delta(\vec{r}_0 - \vec{r}) = \delta(\vec{r}\,' - \vec{r}). \tag{20}$$

The Fourier expansion of a ψ (let us make it time independent for simplicity), in terms of Fourier amplitudes $c_{\vec{r}_0}$, now leads to

$$\psi(\vec{r}) = \int d\vec{r}_0 c_{\vec{r}_0} u_{\vec{r}_0}(\vec{r}) = \int d\vec{r}_0 \psi(\vec{r}_0)\delta(\vec{r} - \vec{r}_0). \tag{21}$$

Now the Fourier coefficients $c_{\vec{r}_0}$, the analogs of the c_n, are just the wave functions $\psi(\vec{r}_0)$. Hence, this description of the state of our system is just the wave function description, where we specify ψ at every point x_0, y_0, z_0 in space time.

To summarize, we have given a number of alternative ways to give a complete description of the state of our system:

1) through specification of Ψ at every point in space time;

2) through the coefficients c_n through an expansion of Ψ in terms of the eigenfunctions of the Hamiltonian of our system;

3) through the coefficients, c_i and $c(\alpha)$, through an expansion of Ψ in terms of the eigenfunctions of an hermitian operator $\overline{H}$ with both a discrete and a continuous eigenvalue spectrum;

4) through the $\phi(\vec{p}, t)$ in a standard Fourier expansion of plane waves.

There are thus many "representations" of our quantum-mechanical system. This will lead us to an introduction to the Dirac notation in the next section.

B The Dirac Notation

Many different "representations" exist that can specify the state of an atomic quantum-mechanical system, described by the wave function, $\Psi(\vec{r}, t)$. We can specify Ψ at every point in space time; we can specify it through the c_n, or through another set c_i and $c(\alpha)$, or through the $\phi(p, t)$, and so on.

Because our $\Psi(\vec{r}, t)$ belong to the space of square-integrable functions, a quantum system specified by a Ψ can be thought of as a vector in infinite-dimensional vector space. The coefficients, c_n, can be thought of as the components of this vector along a particular set of coordinate axes, similarly, for the c_i and $c(\alpha)$ for a different set of coordinate axes. In the same way, the $\phi(\vec{p}, t)$ can be thought of as the components of the state vector along the set of axes specified by the momentum values, and the $\Psi(\vec{r}, t)$ as the components of the state vector along a set of axes specified by the values of the coordinates. The vector space of our Ψ with a well-defined complex scalar product is also called a Hilbert space. Just as in ordinary finite-dimensional vector analysis, it will be convenient to specify a vector by a generic symbol, not always by its coordinates along particular axes. Dirac proposed to do this through his "ket" symbol. Thus, a state vector is specified by $|\Psi\rangle$. Because scalar products $< \Phi, \Psi >$ are complex numbers, linear in Ψ but antilinear in Φ, with

$$\begin{aligned} &< \Phi, (\lambda_1\Psi_1 + \lambda_2\Psi_2) >= \lambda_1 < \Phi, \Psi_1 > + \lambda_2 < \Phi, \Psi_2 >, \qquad \text{but} \\ &< (\lambda_1\Phi_1 + \lambda_2\Phi_2), \Psi >= \lambda_1^* < \Phi_1, \Psi > + \lambda_2^* < \Phi_2, \Psi >, \end{aligned} \tag{22}$$

where λ_1 and λ_2 are complex numbers, Dirac defines for every "ket" vector, $|\Psi\rangle$, a dual vector, the so-called "bra," denoted by $\langle\Psi|$, where

$$\begin{aligned} |\lambda_1\Psi_1 + \lambda_2\Psi_2\rangle &= \lambda_1|\Psi_1\rangle + \lambda_2|\Psi_2\rangle, \\ \langle\lambda_1\Psi_1 + \lambda_2\Psi_2| &= \lambda_1^*\langle\Psi_1| + \lambda_2^*\langle\Psi_2|. \end{aligned} \tag{23}$$

The "bra" vector then permits us to write the scalar product of two vectors in terms of a "bracket"

$$\langle\Phi, \Psi\rangle \equiv \langle\Phi|\Psi\rangle. \tag{24}$$

In the new language, the Hilbert space is an infinite-dimensional vector space of all vectors $|\Psi\rangle$ with a finite norm,

$$\langle\Psi|\Psi\rangle = \text{finite real positive number.}$$

Because we are dealing with an infinite-dimensional vector space, we will also insist on the absolute convergence of expansions, such as

$$\Psi_N = \sum_{n=0}^{N} c_n \psi_n \qquad \text{as} \quad N \to \infty.$$

A linear operator, O, acting on a "ket," $|\Psi\rangle$, converts this into a new "ket," $|\Psi'\rangle = O|\Psi\rangle$, with a dual "bra," given by $\langle\Psi'| = \langle\Psi|O^{\dagger}$, so

$$\langle\Phi|\Psi'\rangle = \langle\Phi|O|\Psi\rangle = \langle\Psi|O^{\dagger}|\Phi\rangle^{*}. \tag{25}$$

$\langle\Phi|\Psi\rangle$ is a number, usually a complex number.

In this new language, an operator can be written as, e.g.,

$$|\Phi\rangle\langle\Lambda| \tag{26}$$

because

$$|\Phi\rangle\langle\Lambda|\Psi\rangle = (\text{a complex number})|\Phi\rangle; \tag{27}$$

that is, the operator $|\Phi\rangle\langle\Lambda|$, acting on the vector $|\Psi\rangle$, converts it into a new vector $|\Phi\rangle$, multiplied by the complex number $\langle\Lambda|\Psi\rangle$.

A very important type of operator is the projection operator, which projects an arbitrary state vector, $|\Psi\rangle$, onto a basis vector, such as $|\psi_n\rangle$. We will assume that $|\psi_n\rangle$ is normalized such that

$$\langle\psi_n|\psi_n\rangle = 1. \tag{28}$$

Then,

$$P_n = |\psi_n\rangle\langle\psi_n|. \tag{29}$$

Note,

$$P_n^2 = |\psi_n\rangle\langle\psi_n|\psi_n\rangle\langle\psi_n| = |\psi_n\rangle\langle\psi_n| = P_n, \qquad \text{via} \quad \langle\psi_n|\psi_n\rangle = 1. \tag{30}$$

Once we have projected the arbitrary vector onto the n^{th} basis vector, projecting once more will not alter this result, so $P_n^2 = P_n$.

The completeness relation for the functions ψ_n can be translated into the "closure" relation in Dirac notation

$$\sum_n |\psi_n\rangle\langle\psi_n| = 1. \tag{31}$$

If the n^{th} energy eigenvalue is degenerate, i.e., if g_n independent eigenfunctions $\psi_n^{(i)}$ with $i = 1, 2, \ldots, g_n$ exist (assuming we have orthonormalized the states with the same n, viz., $\langle\psi_n^{(i)}|\psi_n^{(j)}\rangle = \delta_{ij}$), it may be useful to define a projection operator

$$P_n = \sum_{i=1}^{i=g_n} |\psi_n^{(i)}\rangle\langle\psi_n^{(i)}| \tag{32}$$

that projects onto the subspace of states with definite energy E_n. Now the closure relation (completeness condition) becomes

$$\sum_n \sum_{i=1}^{i=g_n} |\psi_n^{(i)}\rangle\langle\psi_n^{(i)}| = 1. \tag{33}$$

For simplicity, let us for the moment assume no degeneracies exist. Then, P_n acting on an arbitrary state vector $|\Psi\rangle$ yields

$$P_n|\Psi\rangle = |\psi_n\rangle\langle\psi_n|\Psi\rangle = |\psi_n\rangle c_n, \tag{34}$$

or, using the closure relation, an arbitrary state vector, $|\Psi\rangle$, can be expanded in terms of base vectors, $|\psi_n\rangle$,

$$|\Psi\rangle = 1|\Psi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\Psi\rangle = \sum_n |\psi_n\rangle c_n. \tag{35}$$

This equation is the analog in the infinite-dimensional Hilbert space of the expansion of a vector, $\vec{V}$, in ordinary vector analysis in terms of base vectors, $\vec{e}_i$ (unit vectors along the i^{th} direction),

$$\vec{V} = \sum_i \vec{e}_i V_i. \tag{36}$$

If we use some of the other representations introduced in the previous section, we can construct similar projection operators and similar projections. In a basis of eigenvectors of the operator, $\overline{H}$, with

$$\overline{H}|u_i\rangle = E_i|u_i\rangle, \qquad \overline{H}|w_\alpha\rangle = E(\alpha)|w_\alpha\rangle. \tag{37}$$

The closure relation is given by

$$\sum_i |u_i\rangle\langle u_i| + \int d\alpha |w_\alpha\rangle\langle w_\alpha| = 1, \tag{38}$$

and a state vector $|\Psi\rangle$ can be expanded in this basis by

$$|\Psi\rangle = 1|\Psi\rangle = \sum_i |u_i\rangle\langle u_i|\Psi\rangle + \int d\alpha |w_\alpha\rangle\langle w_\alpha|\Psi\rangle = \sum_i |u_i\rangle c_i + \int d\alpha |w_\alpha\rangle c(\alpha). \tag{39}$$

Similarly, in the basis of eigenvectors of the momentum operator, $\vec{p}$,

$$|\Psi\rangle = \int d\vec{p}\,|u_{\vec{p}}\rangle\langle u_{\vec{p}}|\Psi\rangle = \int d\vec{p}\,|u_{\vec{p}}\rangle\phi(\vec{p}, t). \tag{40}$$

Finally, in the basis of eigenvectors of the position operator, $\vec{r}$,

$$|\psi\rangle = \int d\vec{r}_0 |u_{\vec{r}_0}\rangle\langle u_{\vec{r}_0}|\psi\rangle. \tag{41}$$

The projection onto the base vector $|u_{\vec{r}_0}\rangle$ is now just the Schrödinger wave function, $\langle u_{\vec{r}_0}|\psi\rangle = \psi(\vec{r}_0)$, where we have used the orthonormality of the $u_{\vec{r}_0}$, eq. (19).

In all of the above examples, we have expanded ket vectors in terms of ket base vectors. We could of course have done the same with the bra versions of the

vectors. For example, multiplying with the unit operator from the right,

$$\langle\Psi| = \sum_n \langle\Psi|\psi_n\rangle\langle\psi_n| = \sum_n c_n^*\langle\psi_n|. \tag{42}$$

Finally, operators can be represented through their matrix elements via

$$O = 1O1 = \sum_{n,m} |\psi_n\rangle\langle\psi_n|O|\psi_m\rangle\langle\psi_m| = \sum_{n,m} |\psi_n\rangle\langle\psi_m|(O)_{nm}, \tag{43}$$

$$O|\Psi\rangle = \sum_{n,m} |\psi_n\rangle\langle\psi_n|O|\psi_m\rangle\langle\psi_m|\Psi\rangle = \sum_{n,m} |\psi_n\rangle O_{nm}c_m = |\Psi'\rangle = \sum_n |\psi_n\rangle c_n', \tag{44}$$

so

$$c_n' = \sum_m O_{nm}c_m. \tag{45}$$

C Notational Abbreviations

Often, we shall abbreviate the ket $|\psi_n\rangle$ simply by $|n\rangle$. If we have a one-degree of freedom problem, a single quantum number n, associated with the eigenvalue E_n, is sufficient to specify the ket. For a particle moving in three dimensions, three quantum numbers would be needed. For example, for a single particle (without spin) moving in a 3-D harmonic oscillator well, the ket would be specified by $|n_1n_2n_3\rangle$. For a single particle with spin moving in a central potential $V(r)$, the specification $|nlm_lm_s\rangle$ would be natural. Thus, we abbreviate

$$|\psi_n\rangle \quad \rightarrow \quad |nlm_lm_s\rangle. \tag{46}$$

Similarly, for the momentum representation

$$|u_{\vec{p}}\rangle \quad \rightarrow \quad |\vec{p}\rangle = |p_xp_yp_z\rangle, \tag{47}$$

and, in the coordinate representation

$$|u_{\vec{r}_0}\rangle \quad \rightarrow \quad |\vec{r}_0\rangle = |x_0y_0z_0\rangle. \tag{48}$$