COORDINATE AND MOMENTUM REPRESENTATIONS IN QUANTUM MECHANICS

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1. Introduction

On the basis of physical principles having a very general nature, A. Landé [1] has demonstrated that the mathematical structure of quantum mechanics can be derived without having recourse to the introduction of special assumptions of an *ad hoc* type (such as commutation rules governing canonical observables) which are not immediately suggested by our knowledge of the physical world, but which have simply originated as rules which mathematical physicists have discovered by past experience to yield conclusions in conformity with experiment.

In particular, he establishes that the relationship between two representations of the state of a physical system must necessarily be of unitary type, i.e. if the sets of observables being employed as bases for the representations have discrete spectra, so that the system state is specified by vectors having components α_i, α_i' $(i = 1, 2, \cdots)$ in the two representations, then

$$\alpha_i' = \sum_j u_{ij}\alpha_j, \tag{1}$$

$$\alpha_j = \sum_i u_{ij}^*\alpha_i', \tag{2}$$

where u_{ij} are the elements of a unitary matrix and (2) is the transformation inverse to (1), (asterisks indicate that the conjugate complex quantity is to be taken).

Landé also indicates that the well-known fundamental relationship between the coordinate and momentum representations of a particle's state, from which all other representations of the states of physical systems (ignoring spin observables) may be considered to be derived, follows by application of the special principle of relativity when this is supplemented by the assumption that the relationship between these two representations is unitary in character. The purpose of this note is to perform this derivation of the form of this relationship in a comparatively rigorous manner.

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2. Derivation of the relationship

Let x_i $(i = 1, 2, 3)$ be the coordinates of the particle relative to an inertial frame S and let p_i $(i = 1, 2, 3)$ be the corresponding components of its linear momentum. Then, if $\psi(x_1, x_2, x_3) = \psi(x_i)$ is the wave function describing a particular state A of the particle when the coordinate representation is being employed and if $\phi(p_1, p_2, p_3) = \phi(p_i)$ is the wave function describing the same state in the momentum representation, we shall assume that

$$\phi(p_i) = \int u(p_i, x_i)\psi(x_i)dx, \tag{3}$$

$$\psi(x_i) = \int u^*(p_i, x_i)\phi(p_i)dp, \tag{4}$$

determine the form of the unitary transformation (1), (2), appropriate to the case when the observables of the basis possess continuous spectra. In equations (3) and (4), $dx = dx_1 dx_2 dx_3$, $dp = dp_1 dp_2 dp_3$ and the integrations extend over the full range $(-\infty, \infty)$.

In conformity with the special principle of relativity, we shall assume that the form of this relationship is independent of the inertial frame being employed, i.e. the form of the kernel u does not alter if we transform from one inertial frame to another. Consider, therefore, a second inertial frame S' relative to which the particles coordinates are x'_i and its momentum components are p'_i. Then, we have the orthogonal transformation equations

$$x'_i = \sum_{j=1}^{3} a_{ij}x_j + b_i, \tag{5}$$

$$p'_i = \sum_{j=1}^{3} a_{ij}p_j + c_i, \tag{6}$$

where the coefficients a_{ij} are determined by the inclinations of the axes of S' to the axes of S and satisfy the well-known conditions on the elements of an orthogonal matrix. It should here be noted that, although we are appealing to the special principle of relativity, our object is to develop, not Dirac's relativistic theory, but the classical theory of quantum mechanics. In the same way that the fundamental equations of classical Newtonian mechanics are covariant with respect to a Galilean transformation and, as a consequence, are consistent with the special principle of relativity, we are assuming that the classical theory of quantum mechanics exhibits a similar covariance with respect to this type of transformation. The equations (5) and (6) accordingly represent, not a Lorentz transformation, but a Galilean transformation referring to the particular time instant under consideration.

In the x'-representation, let the state A be determined by a wave

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function $\psi'(x'_i)$ and, in the p'-representation, by a wave function $\phi'(p'_i)$. Then, the probability of finding the particle in the neighbourhood of a given point must be the same whether calculated in the S-frame or the S'-frame and hence

$$|\psi| = |\psi'|. \tag{7}$$

Similarly,

$$|\phi| = |\phi'|. \tag{8}$$

Hence we can write

$$\psi' = \psi e^{\iota\alpha}, \quad \phi' = \phi e^{\iota\beta}, \tag{9}$$

where

$$\begin{aligned} \alpha &= \alpha(x_i, a_{jk}, b_l, c_n), \\ \beta &= \beta(p_i, a_{jk}, b_l, c_n). \end{aligned} \tag{10}$$

According to our initial hypothesis,

$$\phi'(p'_i) = \int u(p'_i, x'_i)\psi'(x'_i)dx'. \tag{11}$$

Substituting from the transformation equations (5), (6) and from (9), we get

$$\phi e^{\iota\beta} = \int u(\sum_j a_{ij}p_j + c_i, \sum_j a_{ij}x_j + b_i)\psi e^{\iota\alpha}dx, \tag{12}$$

where

$$\frac{\partial(x'_1, x'_2, x'_3)}{\partial(x_1, x_2, x_3)} = |a_{ij}| = \pm 1. \tag{13}$$

The negative sign must be taken if the orthogonal transformation is indirect; in this case, it is necessary to replace β by $\beta+\pi$ before arriving at equation (12).

It now follows from equations (3) and (12) that

$$\int u(p_i, x_i)\psi(x_i)e^{\iota\beta}dx = \int u(\sum_j a_{ij}p_j + c_i, \sum_j a_{ij}x_j + b_i)\psi(x_i)e^{\iota\alpha}dx, \tag{14}$$

since β is independent of the x_i. This last equation is to be valid for arbitrary wave functions $\psi(x_i)$ which lead to convergent integrals. For this to be so, it is necessary that

$$u(p_i, x_i)e^{\iota\beta} = u(\sum_j a_{ij}p_j + c_i, \sum_j a_{ij}x_j + b_i)e^{\iota\alpha} \tag{15}$$

identically in the variables x_i, p_i and parameters a_{ij}, c_i, b_i. The form of u can now be deduced as follows:

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First, we note that

(16) $$|u(p_i, x_i)| = |u(\sum_j a_{ij}p_j+c_i, \sum_j a_{ij}x_j+b_i)|.$$

Since b_i, c_i are arbitrary, this identity implies that

(17) $$|u(p_i, x_i)| = \text{constant} = u_0.$$

Taking arguments of both sides of the identity (15), we find

(18) $$\theta(p_i, x_i)+\beta = \theta(\sum_j a_{ij}p_j+c_i, \sum_j a_{ij}x_j+b_i)+\alpha,$$

where

(19) $$\theta = \arg u.$$

Differentiating equation (18) partially with respect of p_i and x_j, since α is independent of p_i and β is independent of x_j, it follows that

(20) $$\frac{\partial^2\theta}{\partial p_i\,\partial x_j} = \sum_{r,s}\frac{\partial^2\theta}{\partial p'_r\,\partial x'_s}a_{ri}a_{sj}.$$

The properties of the coefficients a_{ij} enable us to write this relationship in the inverse form

(21) $$\frac{\partial^2\theta}{\partial p'_i\,\partial x'_j} = \sum_{r,s}a_{ir}a_{js}\frac{\partial^2\theta}{\partial p_r\,\partial x_s},$$

from which it is clear that the quantities $\partial^2\theta/\partial p_i\partial x_j$ transform between two rectangular cartesian frames like the elements of a tensor of the second rank.

Putting $x_i = 0$, $p_i = 0$ $(i = 1, 2, 3)$ in the identity (21), we obtain

(22) $$\frac{\partial^2\theta}{\partial c_i\,\partial b_j} = \sum_{r,s}a_{ir}a_{js}\left(\frac{\partial^2\theta}{\partial p_r\,\partial x_s}\right)_0,$$

where the subscript zero indicates that the arguments p_r, x_s are put equal to zero after differentiation. But the right-hand member of equation (22) is independent of c_i and b_j and it follows, therefore, that the left-hand member is also. Thus

(23) $$\frac{\partial^2\theta}{\partial p_i\,\partial x_j} = \chi_{ij},$$

where the χ_{ij} are constants. Equation (21) can now be written

(24) $$\chi_{ij} = \sum_{r,s}a_{ir}a_{js}\chi_{rs},$$

implying that χ_{ij} is a second rank tensor whose elements are the same in every frame. It is shown by H. Jeffreys [3] that any such tensor must be an invariant multiple of the fundamental tensor, i.e.

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(25) $$\chi_{ij} = \gamma\delta_{ij}.$$

We have proved, therefore, that

(26) $$\frac{\partial^2\theta}{\partial p_i\,\partial x_j} = \gamma\delta_{ij}.$$

Integrating, we find that

(27) $$\theta = \gamma\sum_i p_i x_i + P + X,$$

where P is a function of the p_i alone and X is a function of the x_i alone. Hence

(28) $$u = u_0 \exp\{\iota(\gamma\sum_i p_i x_i + P + X)\}.$$

The transformation equations (3), (4) can now be written as

(29) $$e^{-\iota P}\phi(p_i) = \int u_0 e^{\iota\gamma\Sigma p_i x_i} e^{\iota X}\psi(x_i)dx,$$

(30) $$e^{\iota X}\psi(x_i) = \int u_0 e^{-\iota\gamma\Sigma p_i x_i} e^{-\iota P}\phi(p_i)dp.$$

But the only connection between the physical world and the mathematical symbolism is that $|\psi|^2$, $|\phi|^2$ are interpretable as probability densities. This connection is unaltered if we now absorb a factor $e^{\iota X}$ in ψ and a factor $e^{-\iota P}$ in ϕ, to yield new wave functions, which we can then again denote by ψ, ϕ respectively.

γ is a fundamental constant of the physical world and its value can only be decided by comparing the physical implications of equations (29), (30), with actual observations. It is found that the agreement between theory and experiment can only be obtained if we take $\gamma = -1/\hbar$ (the negative sign is purely conventional), where $2\pi\hbar$ is the constant introduced originally by Planck. However, the most fundamental definition of Planck's constant is that it is the constant which arises at equation (25).

Finally, u_0 is determined by the requirement that the equations (29), (30) should be consistent; these equations are essentially those relating a function and its Fourier transform and it follows from the theory of this relationship that $u_0 = h^{-\frac{3}{2}}$. Thus

(31) $$\phi(p_i) = h^{-\frac{3}{2}}\int e^{-\iota\Sigma p_i x_i/\hbar}\psi(x_i)dx,$$

(32) $$\psi(x_i) = h^{-\frac{3}{2}}\int e^{\iota\Sigma p_i x_i/\hbar}\phi(p_i)dp.$$

Having established these transformation equations relating the coordinate and momentum representations of the state of a particle, the development of the theory of the quantum mechanics of a particle can proceed in a

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straightforward manner (see e.g. Tolman [2]). Thus, in the coordinate representation, it now follows directly that the operators representing the observables x_i, p_i are x_i, $-i\hbar\partial/\partial x_i$, and that, in the momentum representation, the corresponding operators are $i\hbar\partial/\partial p_i$, p_i.

References

[1] A. Landé, *New Foundations of Quantum Mechanics* (Cambridge University Press, 1965).
[2] R. C. Tolman, *The Principles of Statistical Mechanics*, Chap. VII (Oxford University Press, 1955).
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