ON THE PRINCIPLE OF SUPERPOSITION IN QUANTUM MECHANICS

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The principle of superposition of states requires that the states of a dynamical system form a linear vector space. This hypothesis of linearity has usually been regarded as a fundamental postulate in quantum mechanics, of a kind that cannot be explained by classical concepts. Indeed, Dirac [2, p. 14] comments that "the superposition that occurs in quantum mechanics is of an essentially different nature from any occurring in the classical theory, as is shown by the fact that the quantum superposition principle demands indeterminacy in the results of observations in order to be capable of a sensible physical interpretation."

It is therefore of interest to examine to what extent and in what form, if any, the principle of superposition might be latent in classical mechanics. This note presents a demonstration of the superposition principle as a consequence of four properties enjoyed by the Hamilton-Jacobi equation of classical mechanics. These properties are:

(a) invariance under transformations of generalized coordinates,

(b) direct additivity of the degrees of freedom,

(c) linearity in the metric,

(d) it is of first order with respect to the time.

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The method applies to systems with quadratic Hamiltonians, which include most of the leading elementary examples upon which the Schrődinger quantum theory was founded [5]. Our results here will be concerned only with the non-relativistic theory.

Let q_i $(i = 1, \ldots, n)$ denote generalized coordinates, and $\dot{q}_i$ the associated velocities. The quadratic form of kinetic energy is taken to be

$$(1) \qquad T = \frac{1}{2} a_{ik} \dot{q}^i \dot{q}^k ,$$

and this positive definite form defines a Riemannian metric by the conventional formula

$$(2) \qquad ds^2 = a_{ik} dq^i dq^k .$$

We define momenta

$$p_i = \frac{\partial T}{\partial \dot{q}_i} = a_{ik} \dot{q}^k ,$$

and construct the Hamiltonian

$$(3) \qquad H = (T+V) = \frac{1}{2} a^{ik} p_i p_k + V ,$$

where $V = V(q^i)$ is the potential energy and a^{ik} the associate contravariant tensor.

For the gradient operator ∇S we have the squared length

$$(4) \qquad (\nabla S)^2 = a^{ik} \frac{\partial S}{\partial q^i} \frac{\partial S}{\partial q^k} = a^{ik} D_i S \, D_k S ,$$

which is an invariant differential expression. Here we use D_i to denote covariant differentiation. The Laplacian

(5) $$\nabla S = \nabla . \nabla S = \frac{1}{\sqrt{a}} \frac{\partial}{\partial q^i} \left(\sqrt{a}\, a^{ik} \frac{\partial S}{\partial q^k} \right),$$

$$= a^{ik} D_i D_k S$$

wherein a denotes the determinant $|a_{ik}|$, is the other basic invariant differential operator related to the metric (2).

The expressions (4) and (5) are the only differential invariants which satisfy (c), i.e., which contain only one contraction over covariant indices. They are also additive in the degrees of freedom of the system in the following "direct" sense. When two systems are considered in conjunction, the Hamiltonians will be added,

(6) $$H = H_1(q^k, p_k) + H_2(q^r, p_r),$$

and the respective metric tensors will be formed into the direct sum

(7) $$(a_{ik}) = \begin{pmatrix} a_{1k\ell} & 0 \\ 0 & a_{2rs} \end{pmatrix}.$$

Likewise the combined phase function

(8) $$S = S_1(q^k) + S_2(q^r)$$

is additive, the separate parts being functions of their respective coordinates. It is then found that the differential invariants (4) and (5) are additive. The Hamilton-Jacobi equation itself also combines additively, in the sense that by adding the component equations we obtain the equation for the combined system.

We now consider how to modify the Hamilton-Jacobi equation

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(9) $$\frac{\partial S}{\partial t} + H \equiv \frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 + V(q) = 0$$

in view of the evidence pertaining to quanta. In searching for a correction term to be added to (9) we insist that the properties (a), (b), (c) and (d) shall be maintained for the modified equation just as for (9). According to (d), we consider only derivatives with respect to the space variables. From (a) and (b), these must appear as combinations of (4) and (5); since the first of these is already present, we are restricted to the Laplacian ΔS as a correction term. By (c), this term must appear linearly. Finally, in order that the additivity property (b) hold, the coefficient in the correction term must be an absolute constant, presumably related to Planck's constant. We therefore take as the extended form of (9)

(10) $$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 + V(q) = \frac{i\hbar}{2}\Delta S ,$$

where $\hbar$ is Planck's constant divided by 2π.

THEOREM 1. (Uniqueness of the singular perturbation.)

Any extension of the Hamilton-Jacobi equation having properties (a), (b), (c) and (d) necessarily takes the form (10), where the coefficient $\hbar$ is a universal constant.

The imaginary factor ensures that the leading derivatives with respect to space and time define a self-adjoint linear differential operator. Though the self-adjoint operator

$$i\frac{\partial}{\partial t} + \frac{\hbar}{2}\Delta$$

is not hyperbolic in the sense of Gårding [3], it is regular according to the definition of Gelfand and Shilov [4, p. 269].

The Hamilton-Jacobi equation (9) is a non-linear partial differential equation of the first order. By constructing a complete integral of (9), we can in turn trace the characteristic curves corresponding to the particle paths in the phase space of coordinates and momenta. These paths are just the integral curves of the Hamiltonian equations of motion.

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The extended Hamilton-Jacobi equation (10) is linear in the highest derivatives of q, t present. However the appearance of the squared gradient term implies its classification as semi-linear. Also this semi-linear regular diffusion equation is a singular perturbation (with parameter $\hbar$) of the classical equation (9), because the highest derivatives disappear in the classical limit. Thus we may expect that solutions of (10) initially concentrated near trajectories of (9) will in some sense diffuse or disperse from them only slowly with the passage of time. Moreover this rate of dispersion will tend to zero with h [1].

THEOREM 2. (Principle of Superposition.) The substitution

(11) $$\psi = e^{iS/\hbar}$$

transforms the extended Hamilton-Jacobi equation (10) to a linear homogeneous equation (12).

The proof follows by actual substitution. We have

$$S = -i\hbar \log \psi$$

or

$$\nabla S = -i\hbar \nabla\psi/\psi ,$$

so that

$$(\nabla S)^2 = -\hbar^2 (\nabla\psi)^2/\psi^2$$

while

$$\Delta S = -i\hbar \frac{\Delta\psi}{\psi} + i\hbar \frac{(\nabla\psi)^2}{\psi^2} ,$$

and

$$S_t = -i\hbar\, \psi_t/\psi .$$

Thus we find

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$$S_t + \frac{1}{2}(\nabla S)^2 + V - \frac{i\hbar}{2}\Delta S$$

$$= -i\hbar\frac{\psi_t}{\psi} - \frac{\hbar^2(\nabla\psi)^2}{2\psi^2} + V - \hbar^2\frac{\Delta\psi}{2\psi} + \frac{\hbar^2(\nabla\psi)^2}{2\psi^2} ,$$

so that ψ satisfies the Schrödinger equation [5, p. 104]

(12) $$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2}\Delta\psi + V\psi .$$

Because this equation is linear and homogeneous, its solutions can be superposed - indeed they form a linear vector space. This concludes our demonstration of the superposition principle in consequence of properties (a), (b), (c), (d).

To any solution of (12) there corresponds an S by (11) and, in the limit $\hbar \to 0$, an action function for the classical system. However, as any wave function or vector ψ can be represented in many ways as a superposition of other vectors (for instance, basis vectors or eigenvectors), we now have reason to consider any given state as being a combination of other states, possibly in many different ways. As Dirac [2, p. 12] comments, the superposition principle "requires us to assume that between these states there exist peculiar relationships such that whenever the system is definitely in one state we can consider it as being partly in each of two or more other states. The original state must be regarded as the result of a kind of superposition of two or more other states, in a way that cannot be conceived on classical ideas. Any state may be considered as the result of a superposition of two or more other states, and indeed in an infinite number of ways. Conversely, any two or more states may be superposed to give a new state."

As remarked above, this is a description of a linear vector space of states. Dirac then goes on to show that in non-relativistic quantum mechanics, "the intermediate character of the state formed by superposition thus expresses itself through the probability of a particular result ... being intermediate." However the probabilistic interpretation of wave functions comes as an observational consequence of the linearity.

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What we have shown in this note, for systems with quadratic Hamiltonians, is that the quantum principle of superposition, though essentially different from any classical superposition, is nonetheless implied by four postulates which are present in classical mechanics.

Because the transition to quantum mechanics is achieved by a singular perturbation, the superposition principle disappears in the classical limit, as is well known. The difficulty of predicting it from classical considerations would therefore be very great, as Dirac quite properly implies. This is, however, a true measure of the insight of Schrödinger [5] and Heisenberg. When faced with the difficulties of the singular perturbation, they made the correct hypothesis of linearity, in spite of its absence from classical mechanics.

REFERENCES

1. L. de Broglie and L. Brillouin, Selected papers on wave mechanics. London, 1928.

2. P. A. M. Dirac, Principles of Quantum Mechanics. 3rd ed., Oxford, 1947.

3. L. Gårding, Linear hyperbolic differential equations with constant coefficients. Acta Mathematica, 85 (1951), 1-62.

4. I. M. Gelfand and G. E. Shilov, Fourier transforms of rapidly increasing functions and questions of the uniqueness of the solution of Cauchy's problem. Uspehi Mat. Nauk (N. S.) 8, (58), (1953), p. 3-54. (A. M. S. trans. ser. 2, vol. 5.)

5. E. Schrödinger, Collected papers on wave mechanics. London, 1928.

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