ON THE SPREADING OF QUANTUM AND CLASSICAL PROBABILITY PACKETS

PHYSICS

1965

SovietRxiv

Abstract

Full Text

UDC 530.1(018)

PHYSICS

Yu. E. MURAKHVER

ON THE SPREADING OF QUANTUM AND CLASSICAL PROBABILITY PACKETS

(Presented by Academician V. A. Fock on 3 IV 1965)

1. By a quantum probability packet (the generally accepted term is wave packet) we shall mean the wave function of a particle or system of particles localized in some region of configuration space. By a classical probability packet we shall mean a statistical ensemble of copies of a given classical system grouped about some mean position in phase space. Various physical objects may serve as realizations of a classical probability packet; we shall mention only two: 1) a system with imprecisely specified initial data and 2) a beam of particles, the interaction between which may be replaced by an effective potential field.

The property of quantum probability packets for a free particle to spread without bound with the passage of time has in fact been known since the emergence of quantum mechanics. In a number of textbooks, for example ([1], [2]), the law of this spreading is derived. The spreading of classical packets is little known, although it has been studied in much greater detail. As early as the beginning of this century Poincaré drew attention to it (for references to his works see ([3])). He also emphasized the importance of this effect for the foundation of statistical physics. This question was considered in detail by N. S. Krylov ([3]). He showed that, for the conclusions of statistical physics to be applicable to a specific mechanical system, it is necessary and sufficient that the latter be a system of the mixing type, i.e., that with time any initial probability distribution should spread uniformly over the layer of univalent integrals of motion. Independently of Krylov, the spreading of classical probability packets was investigated by Born and Houton ([4]-[8]), who used an apparatus more convenient for this purpose from classical statistical mechanics—the Liouville equation for the distribution function in phase space. They proved that in the case of finite motion of arbitrary conservative systems admitting complete separation of variables in the Hamilton-Jacobi method, the uncertainty of the state increases without bound with time. The sole exception is the system of noninteracting harmonic oscillators. Somewhat later the same theorem was proved by Brillouin ([9], [10]) for the finite motion of arbitrary conservative systems.

Thus, in finite motion of conservative systems, mixing inevitably occurs ([5]). Consequently, if the initial distribution corresponds to a specified value of the total energy of the system, then with time it passes into the microcanonical distribution. This is true even for a single particle. Complex systems need be taken into account only if we wish to pass to the canonical distribution ([5]).

The subject of the present note is a comparison of the laws of spreading of quantum and classical probability packets both for finite and for infinite motion in arbitrary potential fields.

2. The time derivative of the mean value of a certain physical-

···quantity F can be calculated in quantum and classical mechanics from the formula $\frac{d}{dt}\overline{F} = \overline{\frac{dF}{dt}}$. In the first case the averaging is carried out over the wave function satisfying the nonstationary Schrödinger equation; in the second, over the distribution function in phase space obeying the Liouville equation. Accordingly, for quantum and classical mechanics we have

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{i}{\hbar}(HF - FH); \tag{1}$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_i \left(\frac{\partial F}{\partial x_i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial x_i} \right), \tag{2}$$

where x_i and p_i are generalized coordinates and momenta, and H is the Hamiltonian of the system.

In deriving the law of spreading, we shall restrict ourselves to the case of one-dimensional motion. We write the Hamiltonian of the problem under consideration in the form $H = p^2/2m + U(x)$. The only approximation that will be admitted in the derivation consists in replacing the potential $U(x)$ by the expression

$$U(x) \approx U(\bar{x}) + U'(\bar{x})(x - \bar{x}) + \frac{1}{2}U''(\bar{x})(x - \bar{x})^2, \tag{3}$$

where $\bar{x}$ is the mean value of the generalized coordinate x (quantum or classical). Therefore the results obtained are exact for potentials depending quadratically on x. For potentials of arbitrary form they are valid if either of the conditions is fulfilled (Δx^2 and Δp^2 are the dispersions of the quantities x and p):

$$|U'''(\bar{x})|\,\Delta x \ll |U''(\bar{x})| \quad \text{or} \quad m|U''(\bar{x})|\Delta x^2 \ll \Delta p^2. \tag{4}$$

Applying (1) to the operator $F = x^2 - \bar{x}^2$ and noting that

$$\frac{d}{dt}(AB) = \frac{dA}{dt}B + A\frac{dB}{dt},$$

we write

$$\frac{d}{dt}\overline{(x^2 - \bar{x}^2)} = \frac{1}{m}\overline{[(p-\bar{p})(x-\bar{x}) + (x-\bar{x})(p-\bar{p})]}. \tag{5}$$

In an entirely analogous way we obtain

$$\frac{d}{dt}\overline{(p^2 - \bar{p}^2)} = -\overline{(p-\bar{p})[U'(x) - \overline{U'(x)}]} - \overline{[U'(x) - \overline{U'(x)}](p-\bar{p})},$$

which, after using (3), leads to the approximate equality

$$\frac{d}{dt}\overline{(p^2 - \bar{p}^2)} \approx -U''(\bar{x})\,\overline{[(p-\bar{p})(x-\bar{x}) + (x-\bar{x})(p-\bar{p})]}. \tag{6}$$

Comparing (5) and (6), we arrive at the first of the equations of interest to us ($v = p/m$):

$$\frac{d\Delta v^2}{dt} = -\frac{1}{m}U''(\bar{x})\frac{d\Delta x^2}{dt}. \tag{7}$$

Proceeding in the same way with the operator $(x-\bar{x})(p-\bar{p}) + (p-\bar{p})(x-\bar{x})$, which appears in (5), we obtain the second equation

$$\frac{d^2\Delta x^2}{dt^2} = 2\Delta v^2 - \frac{2}{m}U''(\bar{x})\Delta x^2. \tag{8}$$

The derivation of these equations for the classical case differs in no way from that given above (in particular, formulas (5) and (6) remain valid),

except for an insignificant simplification connected with the commutativity of physical quantities.

Thus, if one of conditions (4) is fulfilled—which is the case for a very broad class of probability packets—then their spreading in the quantum and classical cases is described by one and the same closed system of differential equations (7) and (8). The coincidence of the quantum and classical laws of spreading supplements the known result that quantum packets of small size move along classical trajectories, but by no means indicates the equivalence of quantum and classical mechanics. In the classical case it is possible to prescribe zero initial data, i.e., solutions with $\Delta x^2 = 0$ and $\Delta v^2 = 0$ are allowed. In quantum mechanics such initial data, and hence the corresponding solutions, are not allowed by the uncertainty relations. To an even greater degree, the specificity of quantum mechanics consists in the use of complex probability amplitudes and in the effects associated with this.

3. The study of the spreading of probability packets with time requires solving the Cauchy problem for the system (7)–(8); preliminarily, of course, one must find the trajectory of the packet center $x = \bar{x}(t)$, solving the corresponding classical problem. We choose the initial conditions as follows:

$$\Delta v^2\big|_{t=0} = \Delta v_0^2, \qquad \Delta x^2\big|_{t=0} = \Delta x_0^2, \qquad d\Delta x^2/dt\big|_{t=0} = 0. \tag{9}$$

The third condition (9), valid for a broad class of initial distributions, is adopted solely for simplicity. It is easy to verify that it does not affect any physically important conclusions.

If U depends quadratically on x, the system (7)–(8) is exact and at the same time admits an exact solution. We shall analyze separately four possibilities: a) free motion, b) a homogeneous field, c) a harmonic oscillator: $U = m\omega^2 x^2/2$, and d) a parabolic potential barrier: $U = -\frac{1}{2}m\omega^2 x^2$. The most general case of a quadratic dependence of U on x reduces to c) or d).

In cases a) and b) our system has the following solution, satisfying the initial conditions (9):

$$\Delta v^2 = \Delta v_0^2, \qquad \Delta x^2 = \Delta x_0^2 + \Delta v_0^2 t^2. \tag{10}$$

For a free particle these formulas were derived earlier ([1,2,4–8]).

For case c) we obtain

$$\Delta x^2 = \frac{1}{2\omega^2}\left(\Delta v_0^2 + \omega^2 \Delta x_0^2\right) - \frac{1}{2\omega^2}\left(\Delta v_0^2 - \omega^2 \Delta x_0^2\right)\cos 2\omega t; \tag{11}$$

$$\Delta v^2 = \frac{1}{2}\left(\Delta v_0^2 + \omega^2 \Delta x_0^2\right) + \frac{1}{2}\left(\Delta v_0^2 - \omega^2 \Delta x_0^2\right)\cos 2\omega t. \tag{12}$$

From (11), (12) it is seen that for the harmonic oscillator there is no spreading: Δx^2 and Δv^2 are periodic functions of t with a period equal to half the period of the oscillator.

In quantum mechanics such a dependence of the variances on time follows directly from the equidistance of the energy spectrum of the harmonic oscillator. The special case considered in Schiff' s book ([11]) corresponds to the initial state (the ground state) for which $\Delta v_0^2 = \omega^2 \Delta x_0^2$.

In classical mechanics, formulas (11), (12) can also be obtained by solving the Liouville equation

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} - \omega^2 x \frac{\partial \rho}{\partial v} = 0$$

for the oscillator. The desired solution with the initial condition $\rho\big|_{t=0} = f(x, v)$ is

$$\rho = f\left(v\cos\omega t - \frac{v}{\omega}\sin\omega t,\; v\cos\omega t + \omega x\sin\omega t\right).$$

If we are interested in a time interval small in comparison with the period of the oscillator ($\omega t \ll 1$), then formulas (11), (12), as was to be expected

as one would expect, coincide with (10):

$$\Delta v^2 = \Delta v_0^2 + O(\omega^2 t^2), \qquad \Delta x^2 = \Delta x_0^2 + \Delta v_0^2 t^2 + O(\omega^2 t^2).$$

One can pass to d) from c) by making in (11), (12) the substitution $\omega \to i\omega$. Consequently, for the parabolic barrier Δx^2 and Δv^2 grow exponentially with time. It is natural to think that a rapid increase of the uncertainties takes place for packets performing infinite motion in any fields that increase sufficiently rapidly at infinity.

Let us consider the most realistic case of infinite motion, when the field vanishes at infinity. Then one can choose initial distributions for which, at an arbitrary instant of time t, one of the conditions (4) will be satisfied, and hence the spreading of quantum and classical probability packets will for all t be described by the same equations. For sufficiently large t, the packets will spread in accordance with formula (10).

4. The main conclusion of the present work concerning the identity of the laws of spreading of quantum and classical probability packets for a broad class of motions, and all its other results, have been obtained for a one-dimensional problem. It is useful to generalize them to multidimensional systems. This would make it possible to apply the corresponding equations to the solution of concrete problems connected with the spreading of particle beams. Such problems arise, for example, in the design of accelerators. In doing so one can pass to such canonical variables that, for each pair of them, the variances satisfy an independent system of differential equations. Let us also note one obvious generalization: equations (7), (8) remain valid if the potential U depends explicitly on time. In this case, however, the conclusions about mixing are, generally speaking, not valid.

The very fact of the spreading of classical probability packets, and still more the coincidence of the quantum and classical equations of spreading, suggest that, contrary to a widely held opinion, this effect is not related to the applicability or inapplicability of the classical approximation. This conclusion is illustrated by concrete examples ([12,13]) from the theory of atomic collisions.

In conclusion, the author expresses his gratitude to Acad. V. A. Fock and Yu. N. Demkov for valuable comments.

Received
24 II 1965

REFERENCES

1. D. I. Blokhintsev, *Fundamentals of Quantum Mechanics*, Moscow, 1961.
2. N. F. Mott, H. S. W. Massey, *The Theory of Atomic Collisions*, Oxford, 1949; N. Mott, G. Massey, *Theory of Atomic Collisions*, Moscow, 1951.
3. N. S. Krylov, *Works on the Foundations of Statistical Physics*, Moscow-Leningrad, 1950.
4. M. Born, Dan. Akad. Wiss., Math.-phys., 30, No. 2 (1955).
5. M. Born, Phys. Blätter, 11, No. 9, 49 (1955).
6. M. Born, D. J. Hooton, Zs. Phys., 142, No. 2, 201 (1955).
7. M. Born, D. J. Hooton, Proc. Cambr. Phil. Soc., 52, No. 2, 287 (1956).
8. M. Born, Zs. Phys., 153, No. 3, 372 (1958); M. Born, UFN, 69, No. 2, 173 (1959).
9. L. Brillouin, Arch. rat. mech. and anal., 5, No. 1, 76 (1960).
10. L. Brillouin, Inform. and Control, 5, No. 3, 223 (1962).
11. L. I. Schiff, *Quantum Mechanics*, N. Y.–Toronto–London, 1955; L. Schiff, *Quantum Mechanics*, Moscow, 1957.
12. M. J. Seaton, Proc. Phys. Soc., 79, No. 6, 1105 (1962).
13. F. J. Smith, Proc. Phys. Soc., 84, No. 6, 889 (1964).

Note: Figure translations are in progress. See original paper for figures.