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Deterministic model equations of motion for quantum mechanics and some new modes of quantum behaviour

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Abstract. In this paper we propose a deterministic basis for quantum mechanics and give equations of motion (derivable from an action principle) which describe deterministic trajectories in an extended space that the quantum events are assumed to follow. By applying the laws of classical probability, namely the conservation of probability along the deterministic trajectories, we derive a probability description which is found to be a generalization of the Schrödinger description with built-in probability interpretation. The generalized description admits of an infinite number of wave functions following coupled set of Schrödinger-like equations while the total probability is given by the sum of the modulus squared of all these wave functions, one of which is identified as the Schrödinger function. If all the functions other than the Schrödinger wave function be neglected the Schrödinger description is retrieved. It is thus concluded that the classical probability not only embraces probability in quantum mechanics but allows other new modes for its propagation.

We thus predict new modes of quantum behaviour and we discuss two situations and propose experiments where these modes could be looked for. Finally, our theory also provides an identification for the quantum of action, $\hbar$.

Keywords. Quantum mechanics; deterministic trajectories; Copenhagen interpretation; hidden variables; classical probability; uncertainty principle; tunnelling; Bohr-Einstein controversy.

1. Introduction

The probability in quantum mechanics has generally been considered to be of a different nature from the classical probability (see, for example Fine (1972) and reference cited therein). While the latter is usually traced to a genuine lack of information, or some information forgone voluntarily (as, for example in statistical mechanics) the former has generally been regarded as intrinsic and 'irreducible' in nature by the followers of the Copenhagen School.

That the nature of probability should be different in two different physical situations is somewhat disconcerting from a conceptual view point. This question is also the essence of the Bohr–Einstein controversy. For, if we regard the probability in quantum mechanics to be of the same nature as the classical probability we are necessarily led to Einstein's view point that the ψ-function in quantum mechanics describes an ensemble of 'similarly prepared' individual systems rather than the individual systems themselves (as insisted upon by the Copenhagen School). With the Copenhagen view point, on the other hand, we are forced to a concept of probability which is entirely peculiar to itself (see, for instance Schrödinger in Przibram 1967).

Rather than accept such a peculiar concept of probability and other conceptual difficulties emanating therefrom, we assume that the probability in quantum mechanics is also of the same nature as the classical probability. This point of view, naturally leads to the so called ' hidden variables ' theories of quantum mechanics. A review of the hidden variables theories put forward so far has been given in the excellent book by Belinfante (1973) and we shall therefore not discuss them here. We present in this paper what may be considered in some sense as a ' hidden variables ' theory, though for reasons to be given later we would prefer not to use this terminology for this theory. It differs from the other ' hidden variables ' theories in a very important respect namely that it explicitly involves the application of the laws of classical probability theory to the individual events in quantum mechanics.

We first give a generalization of the classical equations of motion by introducing an extra angular coordinate which, together with the three position coordinates and corresponding velocity coordinates, specify completely what we term as the *microstate* of an individual system. The generalized equations of motion then describe the time evolution of the microstate along deterministic trajectories in the extended space.

A quantum mechanical state is then represented as an appropriate ensemble of systems following these generalized trajectories in the extended space. We apply the laws of classical probability to the ensemble and derive what turns out to be a generalization of the Schrödinger formalism with a built-in probability interpretation.

2. The state preparation and the quantum mechanical ensemble

One of the distinctive differences between a quantum mechanical system and a classical one lies in the state preparation which precedes any experiment. This consists, in either case, in obtaining a large number (an ensemble) of systems prepared under identical conditions by means of some specified physical processes. These processes essentially serve to fix identical initial conditions for all the members of the ensemble. In the framework of classical mechanics, all the systems in a given experiment follow, ideally speaking, identical courses. This can be expressed by saying that the process of state preparation in classical mechanics is able to fix or control, in principle, all the initial data or alternatively the integrals of motion. Such states are referred to as *dispersion free.*

The quantum mechanical states, on the other hand, are *dispersive.* In spite of being similarly prepared the systems belonging to a quantum state behave quite differently in a given experiment. From the point of view of the classical probability this means that these systems still differ from each other in the initial values of some of the variables which the state preparation processes are not able to control. Following Khinchin (1949) such initial values or integrals of motion are referred to as " free " while those which can be fixed by the state preparation processes, are called " fixed " or " controllable " integrals of motion.

While the controllable integrals of motion completely specify an ensemble representing a quantum mechanical state, the free integrals serve further to specify the microstate of the individual members of the ensemble. The various members of the ensemble belonging to a quantum state would then naturally have the same set of values for the controllable integrals but will have a distribution in the values of the free integrals.

3. Generalized equations of motion for the microstate in the extended space

As we know, the equation of motion of classical mechanics follow from the stationarity of the action S_c,

$$S_c = \int_{t_1}^{t_2} L\, dt \tag{1}$$

where the (classical) Lagrangian, L is considered to be a function of the coordinates $\mathbf{x}_i$ and the velocities $\dot{\mathbf{x}}_i$. In view of the considerations given in section 2, the equations of classical mechanics must be generalized to include the free variables (or the so-called hidden variables in the conventional terminology) so that they describe the motion of an individual quantum system in a higher dimensional space. The microstate of an individual system is thus specified by the totality of the coordinates $\{\mathbf{x}_i, \chi_i\}$ and the corresponding generalized velocities where the χ_i represent the additional (free) variables.

The generalized equation of motion is then postulated to be given by a variational principle similar to (1)

$$S = \int_{t_1}^{t_2} \Lambda\, dt \tag{2}$$

with a generalized Lagrangian Λ of the form

$$\Lambda = \tfrac{1}{2} \sum_i m_i\, \dot{\mathbf{x}}_i^2 + \tfrac{1}{2} \sum_j g_j\, (\{\mathbf{x}_i\}, \{\chi_i\})\, \dot{\chi}_j^2. \tag{3}$$

We shall consider here only a simple case of a particle of mass m and only one free variable χ which we *assume to be an angular coordinate*. Thus let

$$\Lambda = \tfrac{1}{2} m\, \dot{\mathbf{x}}^2 + \tfrac{1}{2} g\, (\mathbf{x}, \chi)\, \dot{\chi}^2. \tag{3a}$$

The stationarity of the action (2) with Λ given by (3a) then gives the following Euler–Lagrange equations for $\mathbf{x}$ and χ:

$$m\, \ddot{\mathbf{x}} = \tfrac{1}{2}\, \dot{\chi}^2\, \frac{\partial g}{\partial \mathbf{x}}\, (\mathbf{x}, \chi) \tag{4a}$$

$$\frac{d}{dt}\, (g\, \dot{\chi}) = \tfrac{1}{2}\, \dot{\chi}^2\, \frac{\partial g}{\partial \chi}. \tag{4b}$$

These equations constitute a generalization of classical mechanics where now it must be emphasized that $\mathbf{x}$ and $\dot{\mathbf{x}}$ do not represent the corresponding variables of the latter. We must now show under what conditions and with what identifications

these equations go over into those of classical mechanics. Note that if Λ is time independent, then the energy is a constant of motion. Thus

$$\mathcal{E} = \dot{\mathbf{x}} \cdot \frac{\partial \Lambda}{\partial \dot{\mathbf{x}}} + \dot{\chi} \frac{\partial \Lambda}{\partial \dot{\chi}} - \Lambda$$

$$= \tfrac{1}{2} m \dot{\mathbf{x}}^2 + \tfrac{1}{2} g \dot{\chi}^2 \tag{5}$$

Thus the energy is numerically equal to the Lagrangian in this case, and is a constant of motion.

4. The classical limit and the origin of dispersion of a quantum state

We assume that the angular coordinate χ is locally cyclic. This means that g is only weakly dependent on χ locally. The implication of this for the trajectory of a particle is that for a given variation of g along the trajectory the change in the χ coordinate is very large compared to the change in the $\mathbf{x}$ coordinates.

We then integrate both sides of eq. (4b) with respect to t and obtain:

$$g \dot{\chi} = \tfrac{1}{2} \int dt \, \dot{\chi} \frac{\partial}{\partial \chi} (g \dot{\chi}) + \epsilon \text{ (const)}. \tag{6}$$

The integral on the right of eq. (6) is a trajectory integral. If, as stated above, the trajectory advances a little along $\mathbf{x}$ while it changes its χ coordinate by a large amount, so that the fractional change in g due to the change in the $\mathbf{x}$ coordinate is small per period of the χ motion, that is,

$$\eta \equiv (g \dot{\chi})^{-1} \dot{\mathbf{x}} \cdot \frac{\partial g}{\partial \mathbf{x}} \ll 1 \tag{7}$$

then the integral in (6) can be considered to be at constant $\mathbf{x}$ and therefore partially with respect to χ. Thus writing $\dot{\chi}\, dt = d\chi$ we get immediately on carrying out the integration

$$g \dot{\chi} = \tfrac{1}{2} g \dot{\chi} + \epsilon$$

or

$$\tfrac{1}{2} g \dot{\chi} = \epsilon. \tag{8}$$

The condition (7), however, is the familiar condition for the variation of g, following the trajectory, to be adiabatic, so that eq. (8) expresses the adiabatic invariance of $\frac{1}{2} g \dot{\chi}$.

It may be noted that $g \dot{\chi}$ is, by definition, the canonical momentum p_χ, corresponding to the coordinate χ. Equation (8) thus expresses the adiabatic invariance of the canonical momentum p_χ

$$p_\chi \equiv g \dot{\chi} = 2 \epsilon. \tag{8a}$$

If the coordinate $\dot{\chi}$ were strictly ignorable or cyclic, $\partial g/\partial \chi$ would be strictly zero and the invariance of $g\dot{\chi}$ following from eq. (4b) would be strict. The equations of motion (4a) and (4b) for $\mathbf{x}$ and χ respectively would be exactly decoupled. If we now eliminate $\dot{\chi}$ from eq. (4a) using eq. (8) we get

$$m\ddot{\mathbf{x}} = \frac{2\epsilon^2}{g^2}\frac{\partial g}{\partial \mathbf{x}} = -\frac{\partial}{\partial \mathbf{x}}\left(\frac{2\epsilon^2}{g}\right). \tag{9}$$

Equation (9) then describes the motion of the $\mathbf{x}$-coordinate of the point mass m. If this motion be identified with a classical motion, then the quantity $2\epsilon^2/g(\mathbf{x})$ can be interpreted as the potential for this motion. The equation of motion (9) can obviously be obtained from the Lagrangian

$$L = \tfrac{1}{2} m\dot{\mathbf{x}}^2 - \frac{2\epsilon^2}{g} \tag{10}$$

as the Euler-Lagrange equation resulting from the stationarity of the reduced action

$$\delta S_c = \delta \int_{t_1}^{t_2} L\, dt = 0. \tag{11}$$

As is shown in the appendix, this reduced action principle can also be obtained directly by incorporating into the original action (2), the constancy of the canonical momentum p_χ as expressed by eq. (8) or (8a). The potential $V = 2\epsilon^2/g$ as viewed from this higher dimensional space, thus appears as a property of the extended space as described by the metric component g.

Note that so long as the adiabatic invariant of eq. (8) and (8a) is a good invariant, the potential function $V \equiv 2\epsilon^2/g$ is well defined and the classical equation of motion (9) is a good description. However, since the invariance of (8) is only adiabatic, departures from classical motion are to be expected and the potential function as an energy would cease to be well defined whenever the conditions for the validity of the adiabatic invariance are violated. We shall show that these departures can be identified with the quantum behaviour and that statistically these are described by a generalized set of Schrödinger equations.

As noted earlier, if the coordinate χ were strictly ignorable or cyclic, the invariance expressed by eq. (8) or (8a) would be exact and the equations for $\mathbf{x}$ and χ would be decoupled. Equation (9) for $\mathbf{x}$ which describes the classical motion with $2\epsilon^2/g$ as the potential would be *exact*. In this case, systems with different initial values for the χ-coordinate but the same initial values for $\mathbf{x}$ and $\dot{\mathbf{x}}$, and, of course, the same initial values for the canonical momentum p_χ, will all follow the same classical trajectory. The coordinate χ can be considered *hidden* from the point of view of the classical motion, since its presence is not manifested in the latter. Very nearly the same behaviour would follow when χ is not strictly cyclic, but the adiabatic invariance expressed by eq. (8) is good.

When χ is not even approximately cyclic, and therefore when the adiabatic invariance of p_χ is appreciably violated in certain regions of space, the motion of the $\mathbf{x}$

coordinate will depart appreciably from the classical motion. These departures from the classical motion are identified with the quantum behaviour. The exact set of eqs (4a) and (4b) are then the proper equations to describe the motion. Now systems with the same initial values for $\mathbf{x}$, $\dot{\mathbf{x}}$ and, p_χ but different ones for χ will, in general, end up with different values for $\mathbf{x}$ and $\dot{\mathbf{x}}$ after the same time interval. From the point of view of the exact motion as governed by the set (4), the variable χ is no more hidden, because a dispersion in its initial value yields, in general, a dispersion in the final values of $\mathbf{x}$ and $\dot{\mathbf{x}}$. This variable may of course, be *free*, if the state preparation is not able to fix definite initial values for it. The dispersion in a quantum state is then a consequence of one or more free variables of the system acquiring a distribution of initial values during the state preparation.

While the set of eqs (4) describe motions involving arbitrarily large departures from adiabatic invariance of p_χ, we stipulate that the departures corresponding to the actual quantum behaviour are not arbitrarily large and the exact motion for $\mathbf{x}$ though different from the classical one, is usually in the neighbourhood of the latter. This means that the adiabatic invariance of p_χ still holds at least approximately.

5. Formulation in terms of classical probability and the Liouville equation for the system

The set of eqs (4a) and (4b) with an appropriate choice for g describes the time evolution of the microstates of the individual systems. As discussed earlier in section 2 a quantum state is an appropriate ensemble of these microstates (or of systems in these microstates). We shall now specify this ensemble corresponding to the quantum state, which we, of course, consider to be a pure state.

We first stipulate that the ensemble corresponding to any pure quantum state is microcanonical in the *initial value* of the adiabatic invariant p_χ as defined in eq. (8a). We further assume that it is microcanonical in also the energy $\mathcal{E}$ of the system. On the other hand, since the angular coordinate χ is *free*, the state preparation will necessarily result in the systems of the ensemble being distributed over the various values of χ. In general, the systems will also be distributed over various values of the variables $\mathbf{x}$ and $\dot{\mathbf{x}}$ at any given time t. Then if f represents the Liouville density in the phase space of the eight variables $(\mathbf{x}, \dot{\mathbf{x}}, p_\chi, \chi)$ at a time t, we have f satisfying the following Liouville equation

$$\frac{\partial f}{\partial t} + \mathbf{v}.\frac{\partial f}{\partial \mathbf{x}} + \dot{\mathbf{v}}.\frac{\partial f}{\partial \mathbf{v}} + \dot{p}_\chi \frac{\partial f}{\partial p_\chi} + \dot{\chi}\frac{\partial f}{\partial \chi} = 0 \tag{12}$$

where $\dot{\mathbf{v}}$ and $\dot{p}_\chi$ are given by eqs (4a) and (4b) respectively. Following the stipulation made at the end of the last section, we shall assume the adiabatic invariance of p_χ to hold and therefore put

$$\dot{p}_\chi = \frac{d}{dt}(g\dot{\chi}) \simeq 0 \tag{13}$$

in eq. (12). Next, from eq. (9) which uses eq. (8a) or (13) we have for $\dot{\mathbf{v}}$

$$m\dot{\mathbf{v}} = -\frac{\partial}{\partial \mathbf{x}}(2\epsilon^2/g). \tag{14}$$

Because of (13) and the nature of the ensemble constructed above (being microcanonical in $p_\chi = 2\epsilon$), the distribution function f is of the form

$$f = \delta(p_\chi - 2\epsilon)\,\hat{f}(\mathbf{x}, \mathbf{v}, \chi, t; p_\chi = 2\epsilon) \tag{15}$$

where $p_\chi = 2\epsilon$ in $\hat{f}$ appears as a parameter. Using (13) and (15), eq. (12) becomes

$$\frac{\partial \hat{f}}{\partial t} + \mathbf{v}\cdot\frac{\partial \hat{f}}{\partial \mathbf{x}} + \dot{\mathbf{v}}\cdot\frac{\partial \hat{f}}{\partial \mathbf{v}} + \dot{\chi}\,\frac{\partial \hat{f}}{\partial \chi} = 0 \tag{16}$$

5.1. *A change of variables*

In order to be able to make a connection with classical mechanics on the one hand and quantum mechanics on the other, it will be found to be useful to change the variables χ to Φ defined by

$$\Phi = \chi - \frac{1}{\epsilon}\int_0^t dt\,\frac{1}{2}mv^2 \tag{17}$$

and transform eq. (16) accordingly. Thus we have

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\Big|_\chi = \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\Big|_\Phi + \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\Phi\,\Big|_\chi\,\frac{\partial}{\partial \Phi}$$

$$= \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\Big|_\Phi - \frac{1}{2}\,\frac{mv^2}{\epsilon}\,\frac{\partial}{\partial \Phi} \tag{18a}$$

and

$$\frac{\partial}{\partial \chi} = \frac{\partial}{\partial \Phi}. \tag{18b}$$

Equation (16) then becomes

$$\frac{\partial \hat{f}}{\partial t} + \mathbf{v}\cdot\frac{\partial \hat{f}}{\partial \mathbf{x}} + \dot{\mathbf{v}}\cdot\frac{\partial \hat{f}}{\partial \mathbf{v}} + \left(\dot{\chi} - \frac{1}{2}\,\frac{mv^2}{\epsilon}\right)\frac{\partial \hat{f}}{\partial \Phi} = 0 \tag{19}$$

where $\hat{f}$ is now considered as a function of $(\mathbf{x}, \mathbf{v}, \Phi, t; \epsilon)$ and $\dot{\chi}$ and $\dot{\mathbf{v}}$ are to be expressed as functions of the new set of variables. These are given essentially by

eqs (8a) and (14) respectively, where g in these expressions still contains χ as an argument. To express χ in terms of the new variables we substitute for $\frac{1}{2}mv^2$ in (17) from the energy relation (5), so that we have

$$2\chi = \Phi + \frac{1}{\epsilon}\mathcal{E}t. \tag{20}$$

The characteristics of eq. (19) are thus given by

$$\dot{\mathbf{x}} = \mathbf{v} \tag{21a}$$

$$\dot{\mathbf{v}} = -\frac{1}{m}\frac{\partial}{\partial \mathbf{x}}\left(\frac{2\epsilon^2}{g}\right) \tag{21b}$$

and

$$\dot{\Phi} = \frac{2\epsilon}{g(\Phi)} - \frac{1}{2}\frac{mv^2}{\epsilon} \equiv -\frac{L}{\epsilon} \tag{21c}$$

where the χ dependence of g is to be transformed by using the relation (20). The variable Φ now serves in place of χ as the free variable. We note that the right hand side of (21c) is $(-L/\epsilon)$, where L is the (classical) Lagrangian of the system [eq. (11)] except for the weak χ (or Φ) dependence of g. This was, in fact, the motivation for the change of variable from χ to Φ.

The above set of eqs (21a)–(21c) constitutes a generalization of the equations of motion of classical mechanics in an adiabatic approximation to the original set (4a) and (4b). It may be noted that the velocity $\dot{\mathbf{x}}$ appearing in the above set is not the same as the velocity in classical mechanics but tends to the latter in the classical limit.

6. Connection with probability in quantum mechanics and equations for the probability amplitudes

An event in an experiment in quantum mechanics is here identified as the end-point of the trajectory of an individual system in this space. The density of trajectory end-points at a certain point $(\mathbf{x}, \mathbf{v}, \Phi; \epsilon)$ of the space at a time t is given by the function $\hat{f}(\mathbf{x}, \mathbf{v}, \Phi, t; \epsilon)$. Since in an experiment one records the density of end-points without regard either to $\mathbf{v}$ or Φ, the total integrated density is given by

$$\begin{aligned} G(\mathbf{x}, t) &= \int d\Phi\, d\mathbf{v}\, \hat{f}(\mathbf{x}, \mathbf{v}, \Phi, t; \epsilon) \\ &= \int d\Phi\, \tilde{f}(\mathbf{x}, \Phi, t; \epsilon). \end{aligned} \tag{22}$$

Since the functions, $\hat{f}$, $\tilde{f}$ represent probabilities, we demand them to be positive definite. We, therefore, write

$$\hat{f}(\mathbf{x}, \mathbf{v}, \Phi, t) = \hat{\psi}^2 \tag{23}$$

where ψ is a real quantity.

Consider now an experiment over the duration of an infinitesimal time interval τ between the times t and $t+\tau$. Thus using eqs (22) and (23) and introducing a δ-function, $\delta(\mathbf{v}-\mathbf{v}')$, we have at the time $t+\tau$

$$\tilde{f}(\mathbf{x}, \Phi_{t+\tau}, t+\tau) = \int d\mathbf{v}\, d\mathbf{v}'\, \hat{\psi}(\mathbf{x}, \mathbf{v}, \Phi_{t+\tau}, t+\tau)$$

$$\delta(\mathbf{v}-\mathbf{v}')\, \hat{\psi}(\mathbf{x}, \mathbf{v}', \Phi_{t+\tau}, t+\tau). \tag{24}$$

From eq. (19), on the other hand, we have for the infinitesimal time interval τ

$$\hat{f}(\mathbf{x}, \mathbf{v}, \Phi_{t+\tau}, t+\tau) = \hat{f}(\mathbf{x}-\mathbf{v}\tau, \mathbf{v}-\dot{\mathbf{v}}\tau, \Phi_{t+\tau}-\dot{\Phi}\tau, t) \tag{25}$$

where $\dot{\mathbf{v}}$ is given by eq. (21b) and $\dot{\Phi}$ by eq. (21c). Equation (25), as also eq. (19) express the conservation of probability in the space of the set of variables $(\mathbf{x}, \mathbf{v}, \Phi)$ this being a hypersurface defined by $p_\chi = 2\epsilon$ in the space of the original set of eight variables. Making use of (23) in (25) we get on taking the square root

$$\hat{\psi}(\mathbf{x}, \mathbf{v}, \Phi_{t+\tau}, t+\tau) = \pm \hat{\psi}(\mathbf{x}-\mathbf{v}\tau, \mathbf{v}-\dot{\mathbf{v}}\tau,$$

$$\Phi_{t+\tau} + L\tau/\epsilon, t) \tag{26}$$

where we have substituted for $\dot{\Phi}$ from eq. (21c).

We now substitute for $\hat{\psi}(\mathbf{x}, \mathbf{v}', \Phi_{t+\tau}, t+\tau)$ from eq. (26) in eq. (24) taking the positive sign. The choice of the positive sign, as we shall see later, is dictated by the obvious requirement that the leading term on the right hand side of eq. (24) should have the same positive sign as the term on the left hand side. We thus have:

$$\tilde{f}(\mathbf{x}, \Phi_{t+\tau}, t+\tau) = \int d\mathbf{v}\, d\mathbf{v}'\, \hat{\psi}(\mathbf{x}, \mathbf{v}, \Phi_{t+\tau}, t+\tau)$$

$$\delta(\mathbf{v}-\mathbf{v}')\, \hat{\psi}(\mathbf{x}-\mathbf{v}'\tau, \mathbf{v}'-\dot{\mathbf{v}}'\tau, \Phi_{t+\tau}+L'\tau/\epsilon, t) \tag{27}$$

where

$$L' = \tfrac{1}{2} m v'^2 - V(\mathbf{x}, \chi, t). \tag{28}$$

Here V is the 'potential' $2\epsilon^2/g$, which now depends on χ through g and its χ-dependence is to be converted into the Φ dependence through the relation (20). To avoid dependence on the half angles as would follow from the relation (20) we assume that the argument of g is 2χ rather than χ.

We recall that χ is an angular coordinate so that any physically significant function must be periodic in χ with a period 2π. Since Φ, as defined by eq. (17) is given additively in terms of χ, periodicity in χ implies periodicity in Φ also. We therefore write a Fourier series for $\hat{\psi}$ with respect to $\Phi_{t+\tau}$

$$\hat{\psi}(\Phi_{t+\tau}) = \sum_n \hat{\Psi}(n)\, e^{in\Phi_{t+\tau}}. \tag{29}$$

We thus use the Fourier expansion for the $\hat{\psi}$ according to (29) in eq. (27) and expand the Fourier coefficients $\hat{\Psi}(\mathbf{x} - \mathbf{v}'\tau, \mathbf{v}' - \dot{\mathbf{v}}'\tau, n, t)$ around the point $(\mathbf{x}, \mathbf{v}', n, t)$ and use the following Fourier representation for the δ-function, $\delta(\mathbf{v} - \mathbf{v}')$:

$$\delta(\mathbf{v} - \mathbf{v}') = \frac{1}{(2\pi)^3} \int d\mathbf{k}\, e^{i\mathbf{k}\cdot(\mathbf{v}-\mathbf{v}')} \tag{30}$$

We then obtain:

$$\tilde{f}(\mathbf{x}, \Phi_{t+\tau}, t+\tau) = \int d\mathbf{v}\, d\mathbf{v}'\, d\mathbf{k} \sum_{n,\,n'} \frac{1}{(2\pi)^3}\, e^{-in'\Phi_{t+\tau}}$$

$$\hat{\Psi}(\mathbf{x}, \mathbf{v}, -n', t+\tau) \Big\{ \hat{\Psi}(\mathbf{x}, \mathbf{v}', n, t)$$

$$- \mathbf{v}'\tau \cdot \frac{\partial \hat{\Psi}(n)}{\partial \mathbf{x}} + \frac{1}{2}\tau^2 \sum_i v_i'^2 \frac{\partial^2 \hat{\Psi}(n)}{\partial x_i^2}$$

$$+ \tau^2 \sum_{i<j} v'_i\, v'_j \frac{\partial^2 \hat{\Psi}(n)}{\partial x_i\, \partial x_j} - \dot{\mathbf{v}}'\tau \cdot \frac{\partial \hat{\Psi}(n)}{\partial \mathbf{v}'} \Big\}$$

$$\exp i\mathbf{k}\cdot(\mathbf{v} - \mathbf{v}')\, \exp in(\Phi_{t+\tau} + L'\tau/\epsilon). \tag{31}$$

Integrating both sides of eq. (31) over $\Phi_{t+\tau}$ we obtain on using the definition (22) for $G(\mathbf{x}, t)$:

$$G(\mathbf{x}, t+\tau) = \sum_n \left(\frac{1}{2\pi}\right)^3 \int d\mathbf{k}\, d\mathbf{v}\, \exp(i\mathbf{k}\cdot\mathbf{v})$$

$$\hat{\Psi}(\mathbf{x}, n, \mathbf{v}, t+\tau) \int d\mathbf{v}'\, \exp(-i\mathbf{k}\cdot\mathbf{v}')\, \exp(\tfrac{1}{2} inmv'^2\tau/\epsilon)$$

$$\sum_{n'} \Big\{ \delta_{nn'} - \frac{in\tau}{\epsilon} \langle n' | V | n \rangle$$

$$- \left(\mathbf{v}'\tau \cdot \frac{\partial}{\partial \mathbf{x}} - \frac{1}{2}\tau^2 \sum_j v_j'^2 \frac{\partial^2}{\partial x_j^2} - \sum_{i<j} \tau^2 v_i' v_j' \frac{\partial^2}{\partial x_i\, \partial x_j} \right) \delta_{nn'}$$

$$+ \frac{\tau}{m} \frac{\partial}{\partial \mathbf{x}} \langle n' | V | n \rangle \cdot \frac{\partial}{\partial \mathbf{v}'} \Big\} \hat{\Psi}(\mathbf{x}, \mathbf{v}', n, t) \tag{32}$$

where we have expanded the exponential involving the Lagrangian as below:

$$\exp(inL'\tau/\epsilon) = \exp in(\tfrac{1}{2}mv'^2\tau/\epsilon - V\tau/\epsilon)$$

$$= \exp(\tfrac{1}{2} inmv'^2\tau/\epsilon)\, [1 - inV\tau/\epsilon + \ldots] \tag{33}$$

and where the matrix element $\langle n' \mid V \mid n \rangle$ is defined as

$$\langle n' \mid V \mid n \rangle = \int_0^{2\pi} d\Phi \exp(-in'\Phi)\, V \exp(in\Phi). \tag{34}$$

The potential V was assumed to have a weak dependence on χ in a quasi-adiabatic approximation. We can thus effect an expansion in terms of the small parameter η as defined by (7) each term of which is Fourier expanded with respect to the angular coordinate χ. We thus have, using formally ϵ in place of η:

$$V(\mathbf{x}, 2\chi, t) = \sum_{\nu} \epsilon^{|\nu|}\, V(\mathbf{x}, \nu, t) \exp(2i\nu\chi). \tag{35}$$

Substituting for χ in terms of Φ using (20) we get

$$\langle n' \mid V \mid n \rangle = \epsilon^{|n'-n|}\, V(\mathbf{x}, n'-n, t) \exp[i(n'-n)\,\hat{\sigma}\tau/\epsilon]. \tag{36}$$

We next introduce in eq. (32) the Fourier expansion of $\hat{\Psi}(\mathbf{x}, n, \mathbf{v}, t)$

$$\hat{\Psi}(\mathbf{x}, n, \mathbf{v}, t) = \left(\frac{1}{2\pi}\right)^3 \int d\mathbf{k} \exp(i\mathbf{k}\cdot\mathbf{v})\, \Psi(\mathbf{x}, n, \mathbf{k}, t). \tag{37}$$

and obtain:

$$G(\mathbf{x}, t+\tau) = \sum_{n'} \int d\mathbf{k}\, d\mathbf{k}' \left(\frac{2\pi\epsilon}{imn'\tau}\right)^{3/2} \exp[-\tfrac{1}{2} i\epsilon(\mathbf{k}-\mathbf{k}')^2/mn'\tau)]$$

$$(2\pi)^{-6}\, \Psi^*(\mathbf{x}, n', \mathbf{k}, t+\tau) \sum_{n} \Bigg\{ \delta_{nn'} \Bigg[1 + \frac{\epsilon}{mn}(\mathbf{k}-\mathbf{k}')\cdot\frac{\partial}{\partial \mathbf{x}}$$

$$+ \frac{1}{2}\tau^2 \left(\frac{\epsilon}{-imn\tau}\nabla^2 - \sum_i \frac{1}{4}(k_i - k_i')^2 \left(\frac{\epsilon}{mn\tau}\right)^2 \frac{\partial^2}{\partial x_i^2}\right.$$

$$\left. + 2\left(\frac{\epsilon}{mn\tau}\right)^2 \sum_{i<j} (k_i - k_i')(k_j - k_j') \frac{\partial^2}{\partial x_i\, \partial x_j}\right)\Bigg]$$

$$- \frac{in\tau}{\epsilon} \langle n' \mid V \mid n \rangle$$

$$\left. - \frac{i\tau}{m}\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{x}} \langle n' \mid V \mid n \rangle \right\} \Psi(\mathbf{x}, \mathbf{k}, n, t) \tag{38}$$

where we have made use of the following integrals:

$$\int dv' \exp(-i\,\mathbf{k}\cdot\mathbf{v}') \exp(\tfrac{1}{2}\,inm\,v'^2\,\tau/\epsilon) \exp(i\,\mathbf{k}'\cdot\mathbf{v}')$$

$$=\left(\frac{2\pi\,\epsilon}{i\,mn\,\tau}\right)^{\frac{3}{2}} \exp\left[-\tfrac{1}{2}\,i\epsilon\,(\mathbf{k}-\mathbf{k}')^2/mn\,\tau\right] \tag{39a}$$

$$\int dv' \exp(-i\,\mathbf{k}\cdot\mathbf{v}')\,\mathbf{v}' \exp(\tfrac{1}{2}\,inm\,v'^2\,\tau/\epsilon) \exp(i\mathbf{k}'\cdot\mathbf{v}')$$

$$=-\frac{\epsilon}{mn\,\tau}(\mathbf{k}-\mathbf{k}')\left(\frac{2\pi\,\epsilon}{imn\,\tau}\right)^{3/2} \exp\left[-\tfrac{1}{2}\,i\,\epsilon\,(\mathbf{k}-\mathbf{k}')^2/mn\,\tau\right]. \tag{39b}$$

$$\int dv' \exp(-i\mathbf{k}\cdot\mathbf{v}')\,v_i^2 \exp(\tfrac{1}{2}inmv'^2\tau/\epsilon) \exp(i\mathbf{k}'\cdot\mathbf{v}')$$

$$=\left[-\frac{\epsilon}{imn'\tau}-\frac{1}{4}\left(\frac{\epsilon}{mn'\tau}\right)^2(k_i-k_i')^2\right]\left(\frac{2\pi\epsilon}{imn\,\tau}\right)^{3/2}$$

$$\exp\left[-\tfrac{1}{2}i\epsilon\,(\mathbf{k}-\mathbf{k}')^2/mn\,\tau\right]. \tag{39c}$$

Note that

$$\lim_{\tau\to 0}\left(\frac{2\pi\,\epsilon}{imn\,\tau}\right)^{3/2} \exp\left[-\tfrac{1}{2}i\epsilon\,(\mathbf{k}-\mathbf{k}')^2/mn\,\tau\right]=(2\pi)^3\,\delta(\mathbf{k}-\mathbf{k}'). \tag{40}$$

Anticipating this limit, and carrying out integration over $\mathbf{k}'$ we get from eq. (38):

$$G(\mathbf{x},\,t+\tau)=\sum_{n'}(2\pi)^{-3}\int d\mathbf{k}\,\Psi^*(\mathbf{x},\,\mathbf{k},\,n',\,t+\tau)$$

$$\sum_{n}\left[\delta nn'\left\{1-\frac{\epsilon\tau}{2imn}\nabla^2\right\}\right.$$

$$\left.-\frac{in\,\tau}{\epsilon}\left(1-\frac{\epsilon\mathbf{k}}{mn}\cdot\frac{\partial}{\partial\mathbf{x}}\right)\langle n'\,|\,\hat{V}\,|\,n\rangle\right]\Psi(\mathbf{x},\,\mathbf{k},\,n,\,t). \tag{41}$$

From eqs (22), (23), (29) and (37), on the other hand we have:

$$G(\mathbf{x},\,t+\tau)=\sum_{n}(2\pi)^{-3}\int d\mathbf{k}\,\Psi^*(\mathbf{x},\,n',\,\mathbf{k},\,t+\tau)\,\Psi(\mathbf{x},\,n',\,\mathbf{k},\,t+\tau). \tag{42}$$

Comparing the two expressions (41) and (42) for $G(\mathbf{x},\,t+\tau)$ we obtain on interchanging the role of n and n':

$$\Psi(\mathbf{x},\,\mathbf{k},\,n,\,t+\tau)=\left[1-\frac{\epsilon\tau}{2imn}\nabla^2\right.$$

$$-\frac{in\tau}{\epsilon}\left(1-\frac{\epsilon}{mn}\,\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{x}}\right)\langle n\,|\,V\,|\,n\rangle\,\Psi\,(\mathbf{x},\mathbf{k},n,t)$$

$$-\frac{i\tau}{\epsilon}\sum_{n'}n'\left(1-\frac{\epsilon}{mn'}\,\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{x}}\right)\langle n\,|\,V\,|\,n'\rangle\,\Psi\,(\mathbf{x},\mathbf{k},n',t). \tag{43}$$

Expanding the left hand side around t and taking the limit $\tau\to 0$ we obtain:

$$i\frac{\epsilon}{n}\frac{\partial\Psi\,(n)}{\partial t}=-\left(\frac{\epsilon}{n}\right)^2\frac{1}{2m}\,\nabla^2\,\Psi\,(n)$$

$$+\left[\left(1-\frac{\epsilon}{mn}\,\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{x}}\right)V(0)\right]\Psi\,(n)$$

$$+\sum_{n'\neq n}\left[\frac{n'}{n}\left(1-\frac{\epsilon}{mn'}\,\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{X}}\right)\langle n\,|\,V\,|\,n'\rangle\right]\Psi\,(n').$$

$$n=1,2,3\ldots. \tag{44}$$

where $\Psi(n)$ stands for $\Psi\,(\mathbf{x},\mathbf{k},n,t)$ and where $V(0)\equiv\langle n\,|\,V\,|\,n'\rangle$ is just the phase averaged part of the 'potential' V. The total probability density $G(\mathbf{x},t)$ from (42) is obtained ss:

$$G\,(\mathbf{x},t)=\sum_{n}\,(2\pi)^{-3}\int d\mathbf{k}\,\Psi^*\,(\mathbf{x},\mathbf{k},n,t)\,\Psi\,(\mathbf{x},\mathbf{k},n,t). \tag{45}$$

Equation (44) represent a set of coupled partial differential equations for the set of functions $\Psi\,(n,\mathbf{k})$ for different values of n and $\mathbf{k}$. Equation (45) expresses the probability expressed, as usual, as the modulus squarred of the wave function $\Psi\,(n,\mathbf{k})$, now generalized as a sum over the varios modes n and $\mathbf{k}$.

If we assume that $\Psi^*\,(\mathbf{x},\mathbf{k},n,t)\,\Psi\,(\mathbf{x},\mathbf{k},n,t)=\delta\,(\mathbf{k}).\ (2\pi)^3\,\tilde{\Psi}^*\,(n)\,\tilde{\Psi}\,(n)$ and that all $\tilde{\Psi}\,(n)=0$ for $n\neq 1$ the set of eqs (44) and (45) reduce to

$$i\epsilon\,\frac{\partial\tilde{\Psi}(1)}{\partial t}=-\frac{\epsilon^2}{2m}\,\nabla^2\,\tilde{\Psi}(1)+V(0)\,\tilde{\Psi}(1) \tag{46}$$

$$G\,(\mathbf{x},t)=\tilde{\Psi}^*\,(1)\tilde{\Psi}(1). \tag{47}$$

The set of eqs (46) and (47) describe completely the Schrödinger formalism of non-relativistic quantum mechanism provided we identify ϵ with $\hbar$ and $V(0)$ with the classical potential. Equations (44) and (45) may thus be considered as constituting a generalization of the usual Schrödinger theory which involves new modes other than the Schrödinger mode for $n\neq 1$, $k\neq 0$ for the propagation of probability. We

shall discuss in section 7 the interpretation and significance of the new modes represented by the functions $\Psi(n, \mathbf{k})$.

7. Discussion

It may be emphasized that the Schrödinger description and its generalization have been obtained as a consequence of the application of the classical probability to individual events. Thus rather than being restrictive in its application, the classical probability not only embraces the probability in quantum mechanics but allows and predicts new modes provided it is applied appropriately to the events in quantum processes.

To understand the complete significance of these new modes would require a careful analysis of these new functions $\Psi(n, \mathbf{k})$ in terms of ensemble that they represent. We consider these questions in section 7.4. Before this we first consider some interesting physical implications of our model to characteristic quantum phenomena like the quantum tunnelling, uncertainty relations and the existence of $\hbar$, the quantum of action.

7.1. *Identification of ϵ with $\hbar$*

An entirely new feature of our theory is that we have given an identification for $\hbar$ as the value of the adiabatic invariant associated with the locally cyclic variable χ that we introduced. It is a general property of adiabatic invariants that so long as the fields in which the particle moves (here the metric component g) vary slowly, the invariance is good. That is, the value of the expression for it remains close to, say, its initial value. In the present case the condition (7) represents such a condition on the slowness of the variation of g. The $\hbar$ is thus identified with the initial value of $\frac{1}{2}g\dot{\chi}=\epsilon$ (eq. (8)). It has been assumed in the above derivation that all the systems of the ensemble have the same value for it.

Sharp variations in the field lead to significant violations of the adiabatic invariance. This property will be found to be an essential physical feature of our formalism in terms of which we would be able to physically explain the characteristic features of the basic quantum phenomena.

As noted earlier, classical equations of motion follow from the set of eqs (4) with the identification of $2\epsilon^2/g$ with the potential, if the adiabatic invariance $\frac{1}{2}g\dot{\chi}=\epsilon$ of (8) is almost exact. This would be so if the metric g is a slowly varying function of x in the sense of condition (7). In that case, the potential V *as an energy* is a well defined quantity in the sense that a well defined separation of energy into the kinetic and potential energies is possible. When g or alternatively the potential V is rapidly varying, however, so that the adiabatic invariance of $\frac{1}{2}g\dot{\chi}$ is violated the potential as an energy ceases to be well defined. Since the quantum effects are known to be more pronounced when the potential varies rapidly, they would appear to be the manifestations of the violation of the adiabatic invariance. We show that this is indeed the case for the two cases discussed below.

Furthermore, numerical calculations of some adiabatic invariants (Hastie *et al* 1969) have shown that they exhibit jump like changes in their values at certain points of space where the metric has certain particular properties, and the sign and the

magnitude of the change depends on the value of the phase angle just before the change. Since the different members of the ensemble representing a quantum state would be distributed over different values of χ, the dispersion in a quantum state would be a consequence of phase dependent interaction and changes in the adiabatic invariant.

7.2. *The uncertainty relations*

We shall now derive the momentum position uncertainty relation in terms of our model. We shall, first of all, like to emphasize that contrary to the widely held misbelief, the uncertainty principle applies to future predictions rather than to the measurements which by definition refer to completed events (see, for instance Feynman *et al* 1963). Correctly interpreted, the uncertainty principle then states that if a position determination of the particle is attempted with a certain precision $\triangle x$, then the knowledge of its momentum after this determination becomes uncertain by an amount $\triangle p \sim h/\triangle x$. This is obviously a probabilistic statement referring to a spread in the values of the momentum p, over an ensemble rather than to the value in any particular case.

Now for a position determination with an accuracy $\lesssim \triangle x$ to be carried out one must use a particle or any other entity whose characteristic range of interaction is $\lesssim \triangle x$. We shall thus identify $\triangle x$ in the uncertainty relation as the characteristic length $\triangle x=(dV/Vdx)^{-1}$ for the potential V with which the particle (whose position is to be determined) interacts during the determination of its position.

Consider now an interaction over a certain length of time $\triangle t$, which involves a change $\triangle \chi$ of the angle χ. If $\triangle v_x$ is the resulting change in the x-component of the particle velocity (consider only a one dimensional case) then assuming no exchange of energy, we have from eq. (5) following the motion

$$mv_x \triangle v_x = -\triangle \chi \frac{d}{d\chi}(\tfrac{1}{2} g\dot{\chi}^2). \tag{48}$$

Again, following the motion we have:

$$\frac{d}{d\chi} = \frac{dx}{d\chi}\frac{d}{dx} = \left(\frac{dx}{dt}\frac{dt}{d\chi}\right)\frac{d}{dx} = \left(\frac{v_x}{\dot{\chi}}\right)\frac{d}{dx}.$$

Using this and $g\dot{\chi}=2\epsilon=2\hbar$ from (8) in eq. (48) we obtain

$$m\triangle v_x = -\hbar\triangle\chi\left(\frac{1}{\dot{\chi}}\frac{d\dot{\chi}}{dx}\right) \tag{49}$$

where we have neglected the nonadiabatic change of $g\dot{\chi}=2\epsilon$ during the interaction. Noting that the potential $V=\epsilon\dot{\chi}$ we have for $\triangle x=[(1/V)(dV/dx)]^{-1}$ discussed above

$$\triangle x = \left(\frac{1}{V}\frac{dV}{dx}\right)^{-1} = \left(\frac{1}{\dot{\chi}}\frac{d\dot{\chi}}{dx}\right)^{-1}.$$

We thus have from (49)

$$m\triangle v_x \triangle x = -\hbar \triangle \chi. \tag{50}$$

Equation (50) thus gives the actual change of $\triangle v_x$ corresponding to a change $\triangle \chi$ in x following the trajectory when $\triangle x$ is the characteristic length of the potential. If we now consider an ensemble of particles (which are subjected to the position determination with the accuracy $\triangle x$), the change $\triangle \chi$ in χ will be centred around a mean value $\overline{\triangle \chi}$ corresponding to the mean, that is, the classical trajectory for which we have on taking the average of (49)

$$m\overline{\triangle v_x} = -\hbar \overline{\triangle \chi}\left(\frac{1}{V}\frac{dV}{dx}\right)^{-1} = -\frac{\hbar \overline{\triangle \chi}}{\overline{\triangle x}}$$

or

$$m\overline{\triangle v_x}\,\triangle x = -\hbar \overline{\triangle \chi} \tag{50a}$$

Subtracting (50a) from (50) we get

$$m\widetilde{\triangle v}_x \triangle x = -\hbar \widetilde{\triangle \chi} \tag{51}$$

where

$$\widetilde{\triangle v}_x = \triangle v_x - \overline{\triangle v_x}$$

$$\widetilde{\triangle \chi} = \triangle \chi - \overline{\triangle \chi} \tag{51a}$$

denote dispersions around the mean values $\overline{\triangle v_x}$ and $\overline{\triangle \chi}$. Note that $\triangle x$ has the same value for all the systems of the ensemble since it represents the accuracy with which the position determination is carried out over the ensemble.

If we now assume $\widetilde{\triangle \chi}$ to be normally distributed over the ensemble according to

$$P(\widetilde{\triangle \chi}) = \frac{1}{\sqrt{2\pi}} \exp\left[-\tfrac{1}{2}(\widetilde{\triangle \chi})^2\right]$$

then squaring eq. (51) and taking the ensemble average we get ($\widetilde{\triangle p_x} = m\widetilde{\triangle v_x}$)

$$\langle(\widetilde{\triangle p_x})^2\rangle\,(\triangle x)^2 = \hbar^2. \tag{52}$$

Extracting the square root we obtain

$$\langle \widetilde{\triangle p_x}\rangle \triangle x = \hbar \tag{53}$$

where we have denoted for simplicity,

$$\langle \widetilde{\Delta p_x} \rangle = [\langle (\widetilde{\Delta p_x})^2 \rangle]^{1/2} \tag{53a}$$

Equation (53) represents the momentum-position uncertainty relation without the inequality sign, where $\langle \widetilde{\Delta p_x} \rangle$ is mean (square root) spread around the classical trajectory value $\overline{\Delta p_x}$. The root mean squared deviation $\langle \widetilde{\Delta p_x} \rangle$ is this inversely proportional to Δx and vanishes only when $\Delta x \to \infty$. Equation (53), it may be emphasized, does not hold for an individual event. Equation (51), on the other hand, holds for the individual event and accordingly $\widetilde{\Delta p_x}$ for any particular event may have any value including zero (for a given Δx) depending on the value of $\widetilde{\Delta \chi}$. But the important point is that $\widetilde{\Delta \chi}$ cannot be limited *controllably* to any preassigned range. This is a consequence, by definition, of the 'free' nature of the variable χ.

7.3. *Tunnelling of potential barriers*

We shall finally discuss how we can understand physically another of the characteristic quantum phenomena, namely the tunnelling of potential barriers, in terms of our model.

As discussed earlier, the potential $V = \epsilon\dot{\chi} = 2\epsilon^2/g$ as an energy is a well defined quantity only when the adiabatic invariance expressed by eq. (8) is almost exact, and thus only so long as g or V is a slowly varying function of position. The energy conservation equation

$$\mathcal{E} = \tfrac{1}{2}mv^2 + V(\mathbf{x}) \tag{54}$$

is then a well defined equation in that a clear separation exists between the kinetic energy $\frac{1}{2}mv^2$ of a particle and what is defined as a potential energy $V(\mathbf{x})$. When, however, the potential V (or alternatively g) varies rapidly like, for instance, a step function appreciable violations of the adiabatic invariance $\frac{1}{2}g\dot{\chi} = \epsilon$ would occur. The potential energy V as a function of x is no more a well defined function. The energy conservation relation (5), namely

$$\mathcal{E} = \tfrac{1}{2}mv^2 + \tfrac{1}{2}g\dot{\chi}^2 \tag{55}$$

rather than the approximate one (54) is then the correct relation to use. Thus if $\Delta\mathbf{v}$ is the change in velocity of a particle corresponding to a change $\Delta\mathbf{x}$ of its coordinate following the motion, then we have

$$\begin{aligned} 0 &= m\mathbf{v} \cdot \Delta\mathbf{v} + (\tfrac{1}{2}g\dot{\chi})\Delta\dot{\chi} + \dot{\chi}\Delta(\tfrac{1}{2}g\dot{\chi}) \\ &= m\mathbf{v} \cdot \Delta\mathbf{v} + \epsilon\Delta\mathbf{x} \cdot \frac{\partial\dot{\chi}}{\partial\mathbf{x}} + \dot{\chi}\Delta\epsilon \\ &= m\mathbf{v} \cdot \Delta\mathbf{v} + \Delta\mathbf{x} \cdot \frac{\partial V}{\partial\mathbf{x}} + \dot{\chi}\Delta\epsilon \end{aligned} \tag{56}$$

where the second term represents the variation of $\frac{1}{2}g\dot{\chi}^2$ holding $\frac{1}{2}g\dot{\chi}=\epsilon$ constant and hence corresponds to the change of the potential energy $V=\epsilon\dot{\chi}$, while the third term represents the change of ϵ itself and hence corresponds to the nonadiabatic change. Equation (54) corresponds to this third term being zero.

Consider now a particle moving in a potential V. Classically, a particle is forbidden at a point $\mathbf{x}$ where its potential energy $V(\mathbf{x})$ exceeds its total energy $\mathscr{E}$, for according to the relation (54) the kinetic energy $\frac{1}{2}mv^2$ becomes negative at such points. According to the exact eqs (55) and (56), however, this need not be so. If for instance, a change $\triangle\mathbf{x}$ of the position of the particle takes it from a classically accessible to a classically forbidden region (which means that $\triangle\mathbf{x}\cdot\epsilon\partial\dot{\chi}/\partial\mathbf{x}=\triangle\mathbf{x}\cdot\partial V/\partial\mathbf{x}>0$ where $v=0$) then eq. (56) could still be satisfied for real values of v by virtue of the term $\dot{\chi}\triangle\epsilon$ which could provide the balance. The term $\dot{\chi}\triangle\epsilon$ represents the violation of the adiabatic invariance. Thus by virtue of the exact energy relations (55) and (56) (or from the point of view of the approximate classical relations, because of the violations of the adiabatic invariance) the particle would appear to 'tunnel' a potential of a height which is greater than the total energy. Since these violations of the adiabatic invariance are more pronounced for sharply varying potentials, the tunnelling would likewise be more pronounced for such potentials. This is again in conformity with the well known characteristics of this quantum effect. Thus once again we see that the quantum effects can be considered as the manifestations of the violation of the adiabatic invariance of eq. (8).

7.4. *Interpretation of the new functions* $\Psi(n, \mathbf{k})$

We have so far made no restriction in the construction of the quantum mechanical ensemble except that it is microcanonical in the initial value of the adiabatic invariant p_χ. The ensemble may be further specified, however, by assigning distributions for the different constants of motion of the system. If a particular constant of motion is ' controllable ' then an appropriate state preparation process will be able to ' project ' a microcanonical ensemble corresponding to the particular constant of motion. More than one integral of motions may be simultaneously ' controllable '. The arguments of the distribution function then group into ' controllable ' and free integrals of motion, or ' isolating ' and ' non-isolating ' integrals to use the language of stellar dynamics.

We may accordingly replace the arguments of the distribution function $\hat{f}(\mathbf{x}, \mathbf{v}, \chi, t; p_\chi)$ of eq. (15) by as many isolating integrals as may exist. Leaving the explicit dependence on $\mathbf{x}$ and χ in tact, we may replace the three components of $\mathbf{v}$ by three time independent integrals of motion, one of which may be chosen to be the total energy given by eq. (5). The other two may or may not be isolating depending on the symmetry of the system.

Assuming the energy to be the only controllable (or isolating) integral, eq. (16) may be transformed accordingly. Since the energy is an integral motion, $\dot{\mathscr{E}}=0$ and the term $\dot{\mathscr{E}}\partial\hat{f}/\partial\mathscr{E}$ would disappear from the transformed equation, yielding

$$\frac{\partial\hat{f}}{\partial t}+\mathbf{v}\cdot\frac{\partial\hat{f}}{\partial\mathbf{x}}+\dot{\chi}\frac{\partial\hat{f}}{\partial\chi}+\dot{\boldsymbol{\Omega}}\cdot\frac{\partial\hat{f}}{\partial\boldsymbol{\Omega}}=0 \tag{57}$$

where Ω is now a two dimensional vector, and $\hat{f}$ is of the form $\hat{f}(\mathbf{x}, \chi, \Omega, t; p_\chi, \mathscr{E})$. If no other isolating integrals exist then the distribution function must be independent of the non-isolating integrals (see for instance Lynden-Bell 1962). Thus $\hat{f}$ must be independent of Ω. Then eq. (57) further reduces to

$$\frac{\partial \hat{f}}{\partial t} + \mathbf{v} \cdot \frac{\partial \hat{f}}{\partial \mathbf{x}} + \dot{\chi} \frac{\partial \hat{f}}{\partial \chi} = 0 \tag{58}$$

The $\dot{\mathbf{v}} \cdot \partial \hat{f}/\partial \mathbf{v}$ term will consequently also be transformed away from eq. (19). As a result of this, eq. (44) will no longer have the term $\sim \epsilon/mn\, \mathbf{k} \cdot \partial/\partial \mathbf{x} \langle n | V | n' \rangle$. The argument $\mathbf{k}$ of the $\Psi(n, \mathbf{k})$ will now also correspond to the Fourier transformation with respect to $\mathscr{E}$ and Ω. Let these variables be named as λ and $\mathbf{k}$ (a two-dimensional vector). Because of the independence of $\hat{f}$ on Ω, $\Psi^*(n, \lambda, \mathbf{k})\, \Psi(n, \lambda, \mathbf{k})$ will be $\tilde{\Psi}^*(n, \lambda)\, \tilde{\Psi}(n, \lambda)\, (2\pi)^2\, \delta(\mathbf{k})$
so that eq. (45) gives

$$G(\mathbf{x}, t) = \frac{1}{2\pi} \sum_n \int d\lambda \tilde{\Psi}^*(n, \lambda) \tilde{\Psi}(n, \lambda)$$

$$= \sum_n \int d\mathscr{E}\, \Psi^*(n, \mathscr{E}) \Psi(n, \mathscr{E}) \tag{59}$$

where $\Psi(n, \mathscr{E})$ is the inverse transform of $\tilde{\Psi}(n, \lambda)$. If the ensemble be micro-canonical in energy, that is $\delta(\mathscr{E} - \mathscr{E}_0)$, we get

$$G(\mathbf{x}, t) = \sum_n \Psi^*(\mathbf{x}, n, \mathscr{E}_0)\, \Psi(\mathbf{x}, n, \mathscr{E}_0) \tag{60}$$

where the $\Psi(\mathbf{x}, n, \mathscr{E}_0)$ obey the equations

$$\frac{i\hbar}{n} \frac{\partial \Psi(n)}{\partial t} = -\left(\frac{\hbar}{n}\right)^2 \frac{1}{2m} \nabla^2 \Psi(n) + V(0)\Psi(n) + \sum_{n \neq n'} \frac{n'}{n} \langle n | V | n' \rangle \Psi(n') \tag{61}$$

First of all we note that if only one of the functions say $\Psi(1)$ were to be non-zero then it implies that the distribution function $\hat{f}$ will be independent of Φ or χ. Conversely, any dependence of $\hat{f}$ on Φ will reflect in some of the functions $\Psi(\mathbf{x}, n)$ being different from zero. Now χ was postulated to be a 'free' variable so that in state preparation the systems of the ensemble are distributed uniformly over χ (modulo 2π). In the p_χ—χ plane of the phase space the points are distributed over a ring of radius equal to $p_\chi = 2\epsilon$. So long as the adiabatic invariant p_χ is well conserved the distribution in χ or alternatively in Φ will remain uniform, and consequently only the function $\Psi(1)$ will be different from zero.

If in certain processes the adiabatic invariant is significantly violated the distribution in χ (or Φ) will tend to depart from uniformity to at least approximately conserve the phase ' volume ' in the p_χ—χ plane. Such a departure from uniformity will then generate functions $\Psi(n)$, with $n \neq 1$. Such effects may be considered as higher order quantum effects which could arise over very short times in processes involving, say, sharp variations of potential in space or/and time. In view of this we may assign explicit magnitudes to the $\Psi(n)$ in eq. (29) and rewrite it as

$$\hat{\psi}(\Phi) = \sum_n \hbar^{|n|-1}\, \hat{\Psi}(n)\, e^{in\Phi} \tag{62}$$

so that

$$G(\mathbf{x}, t) = \Sigma\, \hbar^{2\,(|n|-1)}\, \Psi^*(n)\, \Psi(n) \tag{63}$$

and eq. (61) reads as

$$\frac{i\hbar}{n}\frac{\partial \Psi(n)}{\partial t} = -\left(\frac{\hbar}{n}\right)^2 \frac{1}{2m} \nabla^2\, \Psi(n) + V(0)\, \Psi(n)$$

$$+ \sum_{n' \neq n} \frac{n'}{n}\, \hbar^{(|n'|-1)} \langle n \,|\, V \,|\, n' \rangle\, \Psi(n'). \tag{64}$$

The expansion (62) is similar to other such expansions in other similar situations (see for instance, Rosenbluth and Simon 1965, Rosenbluth and Varma 1967).

Now, since from eq. (36),

$$\langle n \,|\, V \,|\, n' \rangle = \epsilon^{|n'-n|}\, V(\mathbf{x}, n' - n,)\, \exp\, [i\,(n' - n)\, \mathscr{E} t/\hbar] \tag{65}$$

it suggests that for systems microcanonical in the total conservaed energy $\mathscr{E}$ we seek solutions for $\Psi(n)$ in the form

$$\Psi\,(\mathbf{x}, n, t) = \overline{\Psi}\,(\mathbf{x}, n)\, \exp\, (-in\, \mathscr{E} t/\hbar). \tag{66}$$

This rids eq. (64) of the explicit time dependence. This is also the form which is in conformity with the standard form of the solution in the Schrödinger case. With this eq. (64) gives

$$\mathscr{E}\, \overline{\Psi}(n) = -\left(\frac{\hbar}{n}\right)^2 \frac{1}{2m} \nabla^2 \overline{\Psi}(n) + V(0) \overline{\Psi}(n)$$

$$+ \sum_{n' \neq n} \hbar^{\,|n'-n| + |n'| - 1}\, V(\mathbf{x}, n'-n,) \overline{\Psi}(n') \tag{67}$$

We see that the various modes $\Psi(n)$ are rather weakly coupled to each other through terms $\sim \hbar^{\,|n'-n| + |n'|-1}\, V(\mathbf{x}, n'-n)$ where $V(\mathbf{x}, n'-n)$ is the Fourier component

of the potential arising from its weak dependence on **x**. To be sure, both the expansions (35) for V and (62) for $\tilde{\Psi}(\Phi)$ are somewhat arbitrary in assigning the magnitudes to their terms. Nevertheless, the weakness of the coupling would appear to prevail.

Thus, if as an initial condition one starts out with $\Psi(1)\neq 0$, and $\Psi(n)=0$, $n\neq 1$, then in course of time the $\Psi(n)$, $n\neq 1$ may acquire some small non-zero values, if the system goes through a potential sharply varying in space or time.

8. Observability of the new modes

It would be very interesting indeed if one could observe these new modes corresponding to $n=2$, 3, etc. The relative magnitudes of these modes would of course be small in accordance with the relation (63), so that one will have to look for extremely weak effects, whatever the kind of situations one may be considering.

One may consider a host of situations in which the new modes would predict new effects. We shall, here consider only two physically simple situations to see the kinds of new effects that follows. We further consider, for simplicity, the coupling of only two modes Ψ (1) and $\Psi(2)$ and neglect the others because of their weaker coupling. The coupled set of equations for the stationary state are then obtained from eq. (56) as:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(1)+V(0)\Psi(1)+\hbar^2V(1)\Psi(2)=\mathscr{E}\Psi(1)$$

$$-\left(\frac{\hbar}{2}\right)^2\frac{1}{2m}\nabla^2\Psi(2)+V(0)\Psi(2)+\hbar^2V(-1)\Psi(1)=\mathscr{E}\Psi(2). \tag{68}$$

The eigenvalue problem defined by eq. (68) represents weak coupling of the two separate eigenvalue equations for $\Psi(1)$ and $\Psi(2)$:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(1)+V(0)\Psi(1)=\mathscr{E}\Psi(1)$$

$$-\left(\frac{\hbar}{2}\right)^2\frac{1}{2m}\nabla^2\Psi(2)+V(0)\Psi(2)=\mathscr{E}\Psi(2) \tag{69}$$

through the weak coupling term $\sim \hbar^2V$ (1). The eigenvalues of (68) would then be the two sets of eigenvalues of eqs (69) shifted from their positions because of the small coupling.

8.1. *Electron diffraction*

We consider as one example, the case of an electron in the potential field of a crystal lattice. The equation for Ψ (1) being the usual Schrödinger equation gives the usual allowed eigenvalues, given by the Bragg relation (d is the usual lattice spacing)

$$2\,d\sin\theta=\frac{nh}{mv},\quad \mathscr{E}=\tfrac{1}{2}mv^2 \tag{70}$$

Equation (69) for Ψ (2), on the other hand, gives the relation

$$2d \sin \theta = \frac{nh}{2mv} \tag{71}$$

Thus for a given energy $\mathscr{E}$, the particle behaves, according to the Schrödinger mode $\Psi(1)$, as having the usual de Broglie wave length $\lambda = h/mv$. According to the mode Ψ (2) on the other hand, it would behave as having the wave length $\lambda = h/2mv$, that is, half the de Broglie wave length. The probability of such a behaviour (the Ψ (2) mode) is, according to eq. (63) smaller by a fraction proportional to $\hbar^2$. One would accordingly expect the presence of very faint half-odd integral order maxima in the electron diffraction. It will not be possible to estimate precisely the magnitudes of these half order maxima which are forbidden according to the mode Ψ (1), but these should be more pronounced when quantum effects themselves are more pronounced —that is, when the de Broglie wave lengths are comparable to the characteristic length of the potential.

The de Broglie wave length for an electron of about 100 eV is roughly 1 ÅU. A typical lattice spacing of say 2 ÅU would correspond to a de Broglie wave length of an electron of roughly 25 eV. One would thus expect the half-integral order maxima mentioned above to be observed in low energy electron diffraction (LEED). Such faint half integral order maxima have indeed been observed in at least one case—the diffraction from [100] and [110] planes of tungsten (Gervais *et al* 1968) where they have been termed as 'forbidden' and no satisfactory explanation has been offered for their existence. Such half integral order maxima are, of course, strictly forbidden kinematically by the three dimensional reciprocal lattice. Dynamical or multiple scattering effects in the case of low energy electron diffraction are, however, known to give rise to a very large number of non-Bragg peaks at various fractional order like $5\frac{2}{3}$, $6\frac{1}{3}$, $7\frac{2}{3}$, $8\frac{2}{3}$, $9\frac{4}{7}$, etc. (Dvoryankin *et al* 1970). But these fractional order peaks do not lie specifically at half integral order positions as those observed for tungsten. It would therefore appear that multiple scattering could not account for the systematic observation of these half-integral order maxima (for tungsten).

It would be tempting to identify these half integral order maxima with the mode $\Psi(2)$, but one must obviously first rule out all possibilities of explanation in terms of the usual Schrödinger mode Ψ (1). No such explanation has so far been found, however.

8.2. *Atomic spectra*

One may next consider the implications of the mode $\Psi(2)$ (and other modes $n = 3, 4,$ etc.) for the atomic spectra. It will be easy to see that the eigenvalues for the Coulomb potential for the equation for Ψ (2) may be obtained by replacing $\hbar$ by $\hbar/2$ and may be considered to correspond to the charge on the nucleus to be doubled. Thus for the hydrogen atom, the spectrum for the Ψ (2) mode would correspond to that for the ionized helium.

If we now assume that a very small fraction of the hydrogen atoms exist in the state corresponding to Ψ (2) then they should give rise to atomic lines corresponding the spectrum of the ionized helium (neglecting the difference in the electron reduced mass in the two cases). The observations of these lines, if they exist, would pose

severe problems. First of all, these lines are expected to be extremely faint. Furthermore, there may be several other faint lines from impurities, for instance, from molecular hydrogen which may coincide with the lines to be detected. High purity of the atomic hydrogen sample becomes a very severe requirement besides elimination of other background lines. If, however, one could choose an appropriate laser to correspond to one of the new lines to be detected then one can use it to pump the atoms to the excited state which could then decay coherently to give large enough intensity to be detected. This process, which is known as ' laser resonance fluorescence ', has, in fact been used to detect atoms in very small numbers (Fairbank *et al* 1975).

9. Summary and conclusions

The motivation for this work was to find a deterministic basis for non-relativistic quantum mechanics and to see if the latter can be obtained as a probabilistic description of an ensemble of systems following deterministic trajectories. Contrary to the Copenhagen School view point, the probabilistic nature of the description, in this view point, is then a consequence of the lack of information about some of the initial data pertaining to the deterministic trajectories postulated. The investigation at the same time also seeks to clarify whether the probability in quantum mechanics is of a different nature from the classical probability implicitly presumed in the above view point.

We have given a deterministic set of equations of motion in a space extended by introducing an extra angular coordinate. The motion in classical mechanics is identified as the motion of the position coordinate in an adiabatic approximation, while the quantum behaviour of an individual system is identified as the motion of the system in the extended space in the neighbourhood of the adiabatic (that is, classical) motion.

By applying the laws of classical probability to an ensemble of systems in the extended phase space (in particular, the law of conservation of probability along trajectories—the Liouville theorem) we arrive at a probabilistic description which turns out to be a generalization of the Schrödinger description with a built-in probability interpretation. This generalized description admits of an infinite number of wave function $\Psi(n)$, $n = 1, 2, 3\ldots$ which obey a set of coupled Schrödinger-like equations with the total probability density being $|\Psi(n)|^2$ summed over all the modes $n = 1, 2, 3$, etc. In the particular case that all the modes $n \neq 1$ are negligible (as seems to be the case as observed so far) the system of equations reduces to the Schrödinger set. In general, however, the generalized set of equations do predict the existence of other modes $n \neq 1$ for the propagation of probability. It is, therefore, concluded that the classical probability applied appropriately to individual events not only embraces probability in quantum mechanics, but allows for new modes for its propagation.

We have discussed in section 8 two physical situations in which the effects associated with the new modes could be observed. The mode $\Psi(2)$, for instance, would give rise to the presence of half integral orders in the Bragg diffraction of low energy electrons by crystals. Such faint half integral orders have actually been reported, though their identification with $\Psi(2)$ may be premature and must be subject to

further experimental investigation. We have also suggested a method to observe atomic lines associated with the mode Ψ (2).

Finally, another interesting feature of our theory is that we have given an identification for $\hbar$, as the initial value of the adiabatic action invariant associated with the angle variable that we introduced.

Appendix

We wish to show here that the action principle of eq. (11) for the classical equation of motion (9) can be obtained directly from the original action principle of eq. (2) for the generalized equations of motion (4) by incorporating into the latter the constancy of the canonical momentum p_χ.

$$p_\chi = \frac{\partial \Lambda}{\partial \dot{\chi}} = 2\epsilon \tag{A1}$$

where Λ is the Lagrangian given in eq. (3a).

Consider the variation of the action S of eq. (2):

$$\begin{aligned}\delta \int_{t_1}^{t_2} \Lambda\, dt &= \int_{t_1}^{t_2} dt \left[\frac{\partial \Lambda}{\partial \dot{\mathbf{x}}} \cdot \delta\dot{\mathbf{x}} + \frac{\partial \Lambda}{\partial \dot{\chi}}\, \delta\dot{\chi} + \frac{\partial \Lambda}{\partial \mathbf{x}} \cdot \delta\mathbf{x} + \frac{\partial \Lambda}{\partial \chi}\, \delta\chi\right] \\ &= \left[\frac{\partial \Lambda}{\partial \dot{\chi}}\, \delta\chi + \frac{\partial \Lambda}{\partial \dot{\mathbf{x}}} \cdot \delta\mathbf{x}\right]_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \left\{\left[\frac{d}{dt}\left(\frac{\partial \Lambda}{\partial \dot{\mathbf{x}}}\right) - \frac{\partial \Lambda}{\partial \mathbf{x}}\right] \cdot \delta\mathbf{x} \right. \\ &\quad \left. + \left[\frac{d}{dt}\left(\frac{\partial \Lambda}{\partial \dot{\chi}}\right) - \frac{\partial \Lambda}{\partial \chi}\right] \delta\chi \right\}\end{aligned} \tag{A2}$$

where the integration by parts is carried out as usual. According to the usual arguments, the equations of motion follow from here if we demand that: (i) the end-points do not vary and (ii) the variation of S vanishes for *arbitrary* variation ($\delta\mathbf{x}$, $\delta\chi$) of the path between the end-points.

We note that the condition (A1), which we wish to incorporate can be used to obtain χ by a quadrature. As a consequence, the usual condition that the variations vanish at the end-points is violated since $\delta\chi$ is no longer arbitrary. Making use of (A2) and the Euler-Lagrange equation for $\mathbf{x}$ we get

$$\delta \int_{t_1}^{t_2} \Lambda\, dt = \frac{\partial \Lambda}{\partial \dot{\chi}}\, \delta\chi \Big|_{t_1}^{t_2} = 2\epsilon \int_{t_1}^{t_2} \delta\dot{\chi}\, dt = 2\epsilon\, \delta \int_{t_1}^{t_2} \dot{\chi}\, dt \tag{A3}$$

where now $\dot{\chi}$ is to be considered as a function of $\mathbf{x}$ obtained from (A1) or (8) as

$$\dot{\chi} = \frac{2\epsilon}{g} \tag{A4}$$

Using this in (A3) and transposing terms to left hand side:

$$\delta \int_{t_1}^{t_2} dt \left(\Lambda - \frac{4\epsilon^2}{g} \right) = 0 \tag{A5}$$

Equation (A5) thus expresses the reduced action principle for the motion of the x-coordinate with the reduced Lagrangian

$$\begin{aligned} L &= \Lambda - 4\epsilon^2/g \\ &= \tfrac{1}{2} m\dot{x}^2 - \frac{2\epsilon^2}{g} \end{aligned} \tag{A6}$$

where in the expression (3a) for Λ, $\dot{\chi}$ has been eliminated making use of (A4). We thus see that the expression (A6) is identical with the expression (10) for the Lagrangian for the motion of the x-coordinate.

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