Deterministic Quantum Mechanics

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Abstract: Present quantum theory, which is statistical in nature, does not predict joint probability distribution of position and momentum because they are noncommuting. We propose a deterministic quantum theory which predicts a joint probability distribution such that the separate probability distributions for position and momentum agree with usual quantum theory. Unlike the Wigner distribution the suggested distribution is positive definite. The theory predicts a correlation between position and momentum in individual events.

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1. **Introduction.** Present quantum theory does not make definite prediction of the value of an observable in an individual observation except in an eigenstate of the observable. Application of quantum rules to two separated systems which interacted in the past together with a local reality principle (Einstein locality) led Einstein, Podolsky and Rosen\(^1\) to conclude that quantum theory is incomplete. Bell\(^2\) showed that previous proofs of impossibility of a theory more complete than quantum mechanics\(^3\) (inappropriately called hidden variable theory) made unreasonable assumptions; he went on however to prove\(^4\) that a hidden variable theory agreeing with the statistical predictions of quantum theory cannot obey Einstein locality.

Bell’s research was influenced by the construction by De Broglie and Bohm\(^5\) (dBB) of a hidden variable theory which reproduced the position probability density of quantum mechanics but violated Einstein locality for many particle systems. For a single particle moving in one dimension with Hamiltonian

\[
H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x),
\]

and wave function \(\psi(x,t)\), de Broglie-Bohm proposed the complete description of the state to be \(\{\lambda(t), |\psi\rangle\}\), where \(\lambda(t)\) is the instantaneous position of the particle, and its momentum is

\[
\hat{p}_{dBB}(\lambda,t) = m\frac{d\lambda}{dt} = \text{Re} \frac{\psi^\star(-i\hbar \frac{\partial}{\partial x})/(|\psi|^2)}{|x=\lambda|}. \tag{2}
\]

In an ensemble the position density \(\rho(\lambda, t)\) agrees with \(|\psi(\lambda, t)|^2\) for all time. However, Takabayasi\(^6\) pointed out that the joint probability distribution for
position and momentum given by the theory

$$\rho_{\text{BB}}(\lambda, p, t) = |\psi(\lambda, t)|^2 \delta(p - \hat{p}_{\text{BB}}(\lambda, t))$$  \hspace{1cm} (3)$$
does not yield the correct quantum mechanical expectation value of $p^n$ for integral $n \neq 1$. De Broglie\(^5\) stated that these values in his theory “correspond to the unobservable probability distribution existing prior to any measurement” and measurement will reveal different values distributed according to standard statistical quantum mechanical formula. Such a central role for measurement is unsatisfactory if one wishes to apply the dBB theory to closed quantum systems.

Without using hidden variables, Griffiths\(^7\) and Gell-Mann and Hartle\(^8\) introduced joint probability distributions for noncommuting observables at different times in the consistent history approach to quantum theory of closed systems. Wigner\(^9\) had earlier introduced a joint distribution for $x$ and $p$ at the same time,

$$\rho_W(x, p, t) = \int_{-\infty}^{\infty} \frac{dy}{2\pi\hbar} \psi^\ast\left(x + \frac{y}{2}, t\right) \psi\left(x - \frac{y}{2}, t\right) \exp(ipy/\hbar)$$ \hspace{1cm} (4)$$

which yielded the correct quantum probability distributions separately for $x$ and $p$ on integration over $p$ and $x$ respectively. The Wigner distribution cannot however be considered a probability distribution because it is not positive definite, as seen from the fact that the integral

$$\int dx \, dp \, \rho_{W,\psi}(x, p)\rho_{W,\phi}(x, p) = |(\psi, \phi)|^2/(2\pi\hbar)$$
vanishes for two orthogonal states \( \psi, \phi \).

We wish now to propose a deterministic quantum theory of a closed system with the following properties. (We consider in this paper only 1 particle in 1 space dimension).

(i) At each time, the particle has a definite position \( x \) and a definite momentum \( p \).

(ii) The system point in phase space has a Hamiltonian flow with a \( c \)-number causal Hamiltonian \( H_C(x, p, \psi(x,t), t) \) so that in an ensemble of mental copies of the system the phase space density \( \rho(x, p, t) \) obeys Liouville’s theorem

\[
\frac{d\rho(x, p, t)}{dt} = 0. \tag{5}
\]

Here \( \psi(x,t) \) is the solution of the usual Schrödinger equation

\[
i\hbar \frac{\partial \psi(x,t)}{\partial t} = H\psi(x,t) \tag{6}
\]

with \( H \) being the standard quantum mechanical Hamiltonian for the system and \( H_C \) being determined from the following criteria.

(iii) Each pure “causal state”, i.e., a set of phase space points moving according to a single causal Hamiltonian \( H_C \) has phase space density of the deterministic form

\[
\rho(x, p, t) = |\psi(x,t)|^2 \delta(p - \hat{p}(x,t)), \tag{7}
\]

in which \( p - \hat{p}(x,t) = 0 \) not only determines \( p \) as a function of \( x \), but also determines \( x \) as a function of \( p \) at each time (step functions being allowed when
necessary). Eqn. (7) guarantees on integration over \( p \) the correct quantum probability distribution in \( x \) for any real function \( \hat{p}(x,t) \). The function is determined from the requirement that on integration over \( x \), \( \rho(x,p,t) \) should also yield the correct quantum probability distribution in \( p \). That such a determination is possible and unique apart from a discrete 2-fold ambiguity will be a crucial part of the present theory. It is obvious that our \( \hat{p}(x,t) \) will have to be different from the \( \hat{p}(x,t) \) of de Broglie-Bohm theory.

(iv) Since the quantum probability distributions for \( x \) and \( p \) in the statistics of many measurements are exactly reproduced, so are the standard uncertainty relations. However, the correlation between position and momentum in individual events given by \( \hat{p}(x,t) \) is an additional testable prediction of the present theory.

In Secs. II, III we describe the construction of the momentum \( \hat{p}(x,t) \) and the causal Hamiltonian \( H_C \), in Sec. IV applications to simple quantum systems, and in Sec. V conceptual features of the new mechanics.

2. Construction of Joint Probability Distribution of position and momentum. We seek a positive definite distribution of the form (7) where \( \hat{p} \) is a monotonic function of \( x \)

\[
\epsilon \frac{\partial \hat{p}(x,t)}{\partial x} \geq 0, \quad \epsilon = \pm 1
\]  

(8)

The monotonicity property ensures that for a given \( t \), the \( \delta \)-function establishes a one-to-one invertible correspondence between \( x \) and \( p \) whenever
\[ \frac{\partial p}{\partial x} \] is finite and non-zero. The requirement of reproducing the correct quantum probability distribution of \( p \) is that

\[ \int_{-\infty}^{\infty} \rho(x, p, t) dx = \frac{1}{\hbar} |\tilde{\psi}\left(\frac{p}{\hbar}, t\right)|^2, \quad (9) \]

where \( \tilde{\psi}(k, t) \) is the Fourier transform of \( \psi(x, t) \). We substitute the ansatz (7) into (9) and integrate over momentum to obtain

\[ \int_{-\infty}^{p} dp' \int_{p(x', t) \leq p} dx' |\psi(x', t)|^2 \delta(p' - \hat{p}(x', t)) = \int_{-\infty}^{p} \frac{dp'}{\hbar} |\tilde{\psi}\left(\frac{p'}{\hbar}, t\right)|^2. \quad (10) \]

The region \( \hat{p}(x', t) \leq p \) becomes \( x' \leq x \) if \( \epsilon = 1 \), and \( x' \geq x \) if \( \epsilon = -1 \), where \( \hat{p}(x, t) = p \). Thus, we obtain, for \( \epsilon = \pm 1 \),

\[ \int_{-\infty}^{\epsilon x} dx' |\psi(\epsilon x', t)|^2 = \int_{-\infty}^{\hat{p}(x, t)/\hbar} dk' |\tilde{\psi}(k', t)|^2. \quad (11) \]

The left-hand side is a monotonic function of \( x \) which tends to 1 for \( \epsilon x \to \infty \) for a normalized wave function; the right-hand side is a monotonic function of \( \hat{p} \) tending to 1 for \( \hat{p} \to \infty \) (Parseval’s theorem). Hence, for each \( t \), Eq. (11) determines two monotonic functions \( \hat{p} \) of \( x \), one for each sign of \( \epsilon \). (Note that the curve \( \hat{p}(x, t) \) may have segments parallel to \( x \)-axis or \( p \)-axis corresponding to \( \psi(x, t) \) or \( \tilde{\psi}(p/\hbar, t) \) vanishing in some segment). The two curves \( p = \hat{p}_\pm(x, t) \) so determined yield via Eq. (7) phase space densities \( \rho_\pm \), with different causal Hamiltonians \( (H_C)_\pm \) determined below.

\[ \textbf{3. Determination of the Causal Hamiltonian.} \] We view \( \rho(x, p, t) \) as describing an ensemble of system trajectories in the phase space. We saw in the
last section that such a description is possible at each time. We would now like to find a causal Hamiltonian such that the time evolution in phase space implied thereby is consistent with the time dependent Schrödinger equation.

In order that the total number of trajectories is conserved in time we must have the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \dot{x})}{\partial x} + \frac{\partial (\rho \dot{p})}{\partial p} = 0 \quad (12)$$

If the dynamics of the trajectories is of Hamiltonian nature i.e.

$$\dot{x} = \frac{\partial H_C}{\partial p}, \quad \dot{p} = -\frac{\partial H_C}{\partial x} \quad (13)$$

then we have Liouville’s theorem that the phase space density is conserved,

$$\frac{\partial \rho}{\partial t} + \dot{x} \frac{\partial \rho}{\partial x} + \dot{p} \frac{\partial \rho}{\partial p} = 0 \quad (14)$$

i.e.

$$\frac{\partial \rho}{\partial t} + \left( \frac{\partial H_C}{\partial p} \right) \frac{\partial \rho}{\partial x} - \left( \frac{\partial H_C}{\partial x} \right) \frac{\partial \rho}{\partial p} = 0. \quad (15)$$

The $c$-number Hamiltonian $H_C$ describing the causal time evolution of the trajectories in the phase space will be allowed to be different from the usual $q$-number Hamiltonian $H$ describing the time evolution of the Schrödinger wave function $\psi$ according to Eq. (6).

On substituting into Eq. (15) the ansatz (7) discussed in the last section, we obtain

$$\xi \delta(p - \hat{p}) + \frac{\partial}{\partial \delta(p - \hat{p})} (\eta \delta(p - \hat{p})) = 0 \quad (16)$$
where
\[
\xi = \partial|\psi|^2/\partial t + (\partial H_C/\partial p) \partial|\psi|^2/\partial x - \partial \eta/\partial p \\
\eta = -|\psi|^2 \{\partial \hat{p}/\partial t + (\partial \hat{p}/\partial x) \partial H_C/\partial p + \partial H_C/\partial x\}.
\]

We thus need for consistency
\[
\xi = 0 \quad \text{and} \quad \eta = 0 \quad \text{if} \quad p = \hat{p}. \quad (17)
\]

We now specialise to the usual case when \(H\) is given by Eq. (1). We find that this situation is taken care of with the choice of \(H_C(x, p, t)\)
\[
H_C = \frac{1}{2m} (p - A(x, t))^2 + V(x, t). \quad (18)
\]

The causal Hamiltonian is of the Newtonian form apart from the introduction of a vector potential \(A(x, t)\) and allowing the potential \(V(x, t)\) to differ from \(U(x)\). Eqs. (17) lead to the following equations to determine \(V\) and \(A\) (after using Schrödinger eqn. to substitute for \(\partial|\psi|^2/\partial t\)),
\[
-\partial V(x, t)/\partial x = \partial \hat{p}(x, t)/\partial t + (2m)^{-1} \partial (\hat{p}(x, t) - A(x, t))^2/\partial x, \quad (19)
\]
\[
\partial \left[|\psi|^2(\hat{p} - A - mv)\right]/\partial x = 0, \quad (20)
\]

where \(v\) is given by
\[
v(x, t) = \hbar/(2im) \partial ln(\psi/\psi^*)/\partial x \quad (21)
\]
which is just the de Broglie-Bohm velocity. Eq. (20) implies that the quantity in square brackets must be a function of \(t\) alone. We choose this function
of $t$ to be zero in order to avoid a singularity of the vector potential at the nodes of the wave function. We thus obtain

$$A(x, t) = \hat{p}(x, t) - mv(x, t)$$  \hspace{1cm} (22)$$

With the calculation of the causal Hamiltonian thus completed via Eqs. (18), (19) and (22) a consistent Liouville description emerges.

4. Illustrative Examples. (i) Quantum Free Particle. Let the quantum free particle be described by the Gaussian momentum space wave function

$$\tilde{\psi}(p/\hbar, t) = (2\pi)^{-1/4} \exp\left[-(p - \beta)^2/(2\alpha\hbar^2) - ip^2t/(2m\hbar)\right]$$  \hspace{1cm} (23)$$

so that the coordinate space wave function is

$$\psi(x, t) = (\pi\alpha)^{-1/4} (m\alpha/(m + i\alpha\hbar))^{1/2} \exp f,$$

$$f = -(\alpha/2) \left[(x - \beta t/m)^2 - i \left(\frac{\alpha}{m} x^2 + \frac{2\beta x}{\alpha} \frac{\beta^2 t}{m\alpha} \right) \right] / \left(1 + \frac{\alpha^2 \hbar^2 t^2}{m^2}\right).$$  \hspace{1cm} (24)$$

Our procedure yields

$$A = \hat{p} - \beta = \pm \hbar \sqrt{\frac{m^2 \alpha^2}{m^2 + \alpha^2 \hbar^2 t^2}} \left(x - \frac{\beta t}{m}\right),$$  \hspace{1cm} (25)$$

and

$$\partial V/\partial x = \pm (m^2 + \alpha^2 \hbar^2 t^2)^{-3/2} [xt(\alpha^2 + \beta^2 m) \hbar \alpha m]$$  \hspace{1cm} (26)$$

The determination of the causal Hamiltonian is now complete apart from an irrelevant additive function of $t$. Eq. (25) apart from predicting the momentum $\hat{p} = \beta$ at the centre of the wave packet $x = \beta t/m$, also predicts
values of \( \hat{p} \) at other values of \( x \) which the particle may have in individual events. The quantum potentials \( A \) and \( V \) are seen to be proportional to \( \hbar \) in this example.

(ii) Quantum Oscillator. For the minimum uncertainty coherent state of the harmonic oscillator of mass \( m \), angular frequency \( \omega \) and amplitude of oscillation \( a \) we find

\[
\rho(x,p,t) = \sqrt{\frac{m\omega}{\pi\hbar}} \exp \left[-\frac{1}{2} \frac{m\omega}{\hbar} (x - a \cos(\omega t))^2 \right] \delta(p - \hat{p}(x,t)), \tag{27}
\]

where

\[
\hat{p}(x,t) = -m\omega a \sin(\omega t) \pm m\omega (x - a \cos(\omega t)), \tag{28}
\]

and

\[
A(x,t) = \pm m\omega (x - a \cos(\omega t)), \tag{29}
\]

\[
-\partial V(x,t)/\partial x = -m\omega^2 a \cos(\omega t) \pm m\omega^2 a \sin(\omega t) \tag{30}
\]

The causal Hamiltonian yields the equation of motion

\[
md^2x/dt^2 = -m\omega^2 a \cos \omega t \tag{31}
\]

which results in exact harmonic motion even for \( x \) away from the centre of the packet. We do not of course expect this for solutions of the Schrödinger eqn. different from the coherent state here considered.

5. **New conceptual features.** (a) We have derived corresponding to every quantum wave function \( \psi \), two joint probability distributions for position and
momentum of the form (7) which are (i) positive definite, (ii) have Hamiltonian evolution with causal Hamiltonians \( (H_C)_\pm \) and obey (iii)

\[
\int (f(x) + g(p)) \rho_\pm(x, p, t) dx \, dp = \left( \psi, \left( f(x) + g \left( -i\hbar \frac{\partial}{\partial x} \right) \right) \psi \right),
\]

for arbitrary functions \( f(x) \) and \( g(p) \). Eq. (32) is the major advantage of the present theory over the \( dBB \) theory. It raises the exciting possibility that the momentum values \( \hat{p}_\pm(x, t) \) for individual events here derived could agree with experimental values, and the single particle theory described could be the seed of a general quantum theory of closed systems. We postpone the discussion of measurements until we present a generalization of the theory to many particles.

(b) Since both \( \rho_+ \) and \( \rho_- \) obey Eq. (32) so will \( \rho = C\rho_+ + (1 - C)\rho_- \) with \( 0 \leq C \leq 1 \). But since \( \rho_+ \) and \( \rho_- \) correspond to different causal Hamiltonians \( (H_C)_\pm \), \( \rho \) will not correspond to a ‘pure causal state’. We are led to the concept of a pure causal state as being more fine grained than a pure wave function \( \psi \). All \( \rho = C\rho_+ + (1 - C)\rho_- \) correspond to \( \psi \) (\( \rho \leftrightarrow \psi \)) for a continuum of values of \( C \); but only \( C = 0, 1 \) correspond to pure causal states. To quantum density matrix states \( \Sigma C_\alpha |\psi_\alpha\rangle \langle \psi_\alpha| \) correspond phase space densities \( \Sigma C_\alpha \rho_\alpha \) if \( \rho_\alpha \leftrightarrow \psi_\alpha \).

(c) It is clear that the causal Hamiltonian evolution of phase space densities could be described purely in the phase space language without using the intermediate step of the wave function. We find it convenient to use \( \psi(x, t) \) at the present stage.
(d) One can ask if Eq. (32) can be generalized to more general quantum observables. Here we face the old problem that there exist nonclassical observables e.g. \( x \left( -i\hbar \frac{\partial}{\partial x} \right) x, \left( -i\hbar \frac{\partial}{\partial x} \right) xx + h.c. \) / 2 which have different expectation values but the same ‘naive’ classical analogue \( x^2 p \). A trivial way followed already for the \( dBB \) distribution is: given a nonclassical observable \( A \) the phase space analogue can be \( f(x, p, \psi) \) such that \( f(x, \hat{p}, \psi) = \psi^* A \psi / |\psi|^2 \). Perhaps only those operators \( A \), which like \( (f(x) + q(p)) \) have a phase space representation \( f(x, p) \) independent of \( \psi \) should be considered as ‘beables’.10

(e) The predictions of the momentum values \( \hat{p}(x, t) \) are independent of any special ansatz for \( H_C \).

(f) Due to the existence of trajectories, the problem of inconsistent histories will not arise in this theory.

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