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On the phase-space picture of quantum mechanics

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Abstract

A quantum particle with potential energy $V(\hat{q}, t)$ is considered in the frame of a phase-space picture of the quantum theory, and the interconnection between quantum mechanics and a $\hbar$-dependent *extended classical dynamics* is analysed. The initial position-space wavefunction determines the initial conditions for a set of Hamilton-like equations that leads up to an ensemble of complex-valued phase-space trajectories. The one-dimensional driven harmonic oscillator is used for illustrating the method, and for generating a complete set of phase-space functions.

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1. Introduction

Many authors have investigated the relation between quantum mechanics (QM) and classical mechanics (CM). Among the attempts to formulate both theories in terms of a common language are the Bohmian theory [1–5], the Wigner function [6], the Husimi function [7], a set of phase-space quasi-probability distribution functions [8–13], the stochastic quantum mechanics [14] and the quantum mechanics on phase-space approach [15]. See also references within the cited literature.

To construct the QM–CM bridge there are a number of difficulties to overcome. On the one hand, the two theories have disparate physical and mathematical formulations. For instance: (i) phase-space trajectory is a well-defined classical concept, whereas the Heisenberg uncertainty relation for position and momentum precludes within quantum theory the notion of classical trajectories from the standpoint of the spectral projectors for position and momentum operators. (ii) Hamiltonian dynamics simultaneously involves both position and momentum variables, while the Schrödinger picture of QM only requires either the position or the momentum representation. On the other hand, according to the correspondence principle, in the case of spinless particles QM must agree with CM in some appropriate limit (e.g. $\hbar \to 0$, high quantum numbers, great masses). But the nature of that limiting process is not

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fully understood, and no commonly accepted definition of the correspondence principle yet exists [16].

The focal point of the present paper is to explore some of the characteristics of the QM–CM bridge by starting from the so-called phase-space picture of the QM [17]. The strong point of this is that it follows the conventional approach of quantum-mechanical transformation theory for relating different pictures to each other (e.g. Schrödinger, Heisenberg, interaction).

1.1. System, notation and contents

The physical system. For simplicity, we will consider a quantum particle of mass m with three degrees of freedom, with position and momentum operators $\hat{q} = \{\hat{q}_1, \hat{q}_2, \hat{q}_3\}$ and $\hat{p} = \{\hat{p}_1, \hat{p}_2, \hat{p}_3\}$, and Hamiltonian $H(\hat{q}, \hat{p}, t) = \hat{p}^2/(2m) + V(\hat{q}, t)$, where $V(\hat{q}, t)$ is the potential energy. The Schrödinger equation $\mathrm{i}\hbar(\mathrm{d}/\mathrm{d}t)|\psi(t)\rangle = H(\hat{q}, \hat{p}, t)|\psi(t)\rangle$, with initial state $|\psi(t_o)\rangle$, describes the time evolution of the quantum-mechanical state $|\psi(t)\rangle$. The Hilbert space of the quantum-mechanical states of the particle is designated by $\mathcal{H}$.

We will assume the phase space $\mathcal{H}_{cl}$, with states $(Q, P) := (Q_1, Q_2, Q_3, P_1, P_2, P_3)$. The *coordinates* $Q = Q(t) = Q' + \mathrm{i}Q''$ and *momenta* $P = P(t) = P' + \mathrm{i}P''$ are in general differentiable functions of time t and complex-valued, and the initial values are denoted by $Q_0 := Q(t_0)$ and $P_0 := P(t_0)$. Operators for $\mathcal{H}_{cl}$ are distinguished by a circumflex ($\breve{}$), and we define commuting phase-space operators $\breve{Q} = (\breve{Q}_1, \breve{Q}_2, \breve{Q}_3)$ and $\breve{P} = (\breve{P}_1, \breve{P}_2, \breve{P}_3)$,

$$\breve{Q}_n := \mathrm{i}\hbar\frac{\partial}{\partial P_n} \qquad \breve{P}_n := -\mathrm{i}\hbar\frac{\partial}{\partial Q_n} \qquad n = 1, 2, 3. \tag{1}$$

A multi-index notation is also used: let k be an ordered set $k = (k_1, k_2, k_3)$ consisting of three non-negative integers restricted by $k = k_1 + k_2 + k_3$, then $k! = k_1!k_2!k_3!$, $\breve{Q}^k = \breve{Q}_1^{k_1}\breve{Q}_2^{k_2}\breve{Q}_3^{k_3}$, $(\partial/\partial Q)^k = (\partial/\partial Q_1)^{k_1}(\partial/\partial Q_2)^{k_2}(\partial/\partial Q_3)^{k_3}$, and so on.

The contents of this paper. In section 2 we will briefly outline the basic equations which serve as the starting point for this work. In section 3, we will demostrate that a set of $\hbar$-dependent Hamilton-like equations can be identified allowing the description of complex-valued trajectories $(Q(t), P(t))$ in the phase space $\mathcal{H}_{cl}$, and that the initial conditions of such trajectories are fixed by the initial position-space wavefunction $\psi(x, t_0)$. In section 4, we will be concerned with a procedure for extracting the position and momentum wavefunctions from the phase-space wavefunction $\psi(Q, P, t)$, and with a semiclassical approximation that fully describes the quantum evolution of $\psi(Q, P, t)$ in terms of the phase-space trajectories $(Q(t), P(t))$. In section 5 we will illustrate the theory by dealing with a one-dimensional driven oscillator. Finally, our concluding remarks are summarized in section 6.

2. The basic equations for this work

2.1. Position-space wavefunction in the polar form

Since the position-space wavefunction $\psi(x, t)$ is a complex function, it can be expressed in the polar form

$$\psi(x, t) := \langle x\,|\psi(t)\rangle = R(x, t)\exp\left[\frac{\mathrm{i}}{\hbar}\mathcal{W}(x, t)\right] \tag{2}$$

with the amplitude $R(x, t)$ and the phase $\mathcal{W}(x, t)$ being functions with real values, likewise the position parameter $x := (x_1, x_2, x_3) \in \Re^3$. Thus, inserting (2) into the Schrödinger equation and separating into real and imaginary parts, we obtain that the time-dependent Schrödinger equation is equivalent to the couple of equations [2, 3, 13]

$$\frac{\partial \mathcal{W}(x,t)}{\partial t} + \frac{1}{2m}[\nabla \mathcal{W}(x,t)]^2 - \frac{\hbar^2}{2m}\frac{\nabla^2 R(x,t)}{R(x,t)} + V(x,t) = 0 \tag{3a}$$

$$\frac{\partial R^2(x,t)}{\partial t} + \frac{1}{m}\nabla \cdot [R^2(x,t)\nabla \mathcal{W}(x,t)] = 0 \tag{3b}$$

where the term $V_R(x,t) := -(\hbar^2/2m)(\nabla^2 R(x,t))/R(x,t)$ is the so-called Bohmian quantum potential [2, 5]. It is determined by the amplitude $R(x,t)$ of the wavefunction which in turn depends on the interaction potential $V(x,t)$ and the initial state $\psi(x,t_0)$.

Equation (3*a*) establishes that the phase $\mathcal{W}(x,t)$ of the position-space wavefunction of a quantum particle satisfies an equation of motion that is identical in form to the usual classical Hamilton–Jacobi equation (CHJ), differing from it only by the appearance of the Bohmian quantum potential $V_R(x,t)$ alongside the classical potential energy term $V(x,t)$. However, as annotated in [4], there are also important physical differences between (3*a*) and the CHJ. Equation (3*b*) is the equation of continuity for the probability density $\rho(x,t) := R^2(x,t) = |\psi(x,t)|^2$ of the particle in position space.

2.2. Phase-space picture of quantum mechanics

Consider the specific case in which we restrict the Hamilton operator to $H(\hat{q},\hat{p},t) = \hat{p}^2/(2m) + V(\hat{q},t)$ and the *arbitrary smooth phase-space function* $S(Q,P,t)$ to $S(Q,P_0,t)$. As a result the *auxiliary functions* defined in equation (14) of [17] simplify to $q(Q,P_0,t) := Q$ and

$$p(q,P_0,t) := \frac{\partial S(Q,P_0,t)}{\partial Q}. \tag{4}$$

Next we define in the Hilbert space $\mathcal{H}$ a *phase-space picture* of the Schrödinger equation by the transformation (see equation (41) of [17])

$$|\psi(Q,P,t)\rangle := \exp\left(-\frac{\mathrm{i}}{\hbar}[S(Q,P_0,t) - QP/2]\right)\hat{D}(-Q,-P)|\psi(t)\rangle \tag{5}$$

where $\hat{D}(\pm Q,\pm P) := \exp(\pm(\mathrm{i}/\hbar)[P\hat{q} - Q\hat{p}])$ are the Weyl operator and its inverse.

After expanding $V(q+\breve{Q},t)$ in a Taylor series, and by selecting a suitable choice of the free parameters $\{S,Q,P\}$, the following basic equations emerge [17]:

(i) The *generalized Hamilton equations* (GH)

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \frac{p}{m} = \frac{1}{m}\frac{\partial S(Q,P_0,t)}{\partial Q} \qquad \frac{\mathrm{d}P}{\mathrm{d}t} = -\frac{\partial V(Q,t)}{\partial Q}. \tag{6}$$

(ii) The *quantum Hamilton–Jacobi equation* (QHJ)

$$\frac{\partial S(Q,P_0,t)}{\partial t} + \frac{1}{2m}\left[\frac{\partial S(Q,P_0,t)}{\partial Q}\right]^2 - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 S(Q,P_0,t)}{\partial Q^2} + V(Q,t) = 0 \tag{7}$$

with the initial condition $S(Q,P_0,t_0) = p(Q_0,P_0,t_0)Q$.

(iii) The phase-space representative of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(Q(t),P(t),t)\rangle = \breve{\mathcal{D}}|\psi(Q(t),P(t),t)\rangle \tag{8}$$

with the initial state $|\psi(Q_0,P_0,t_0)\rangle$, and the phase-space operator

$$\breve{\mathcal{D}} = \mathcal{D}(Q,\breve{Q},\breve{P},t) := \frac{1}{2m}\breve{P}^2 + \sum_{k=2}^{\infty} V_k(Q,t)\breve{Q}^k. \tag{9}$$

The symbol $V_k(Q,t)$ is defined for the multi-index $k := (k_1,k_2,k_3)$, and by the relation $k!V_k(Q,t) := (\partial/\partial Q)^k V(Q,t)$.

One can rewrite (8) as an equation with time-independent parameters Q and P by using $\mathrm{i}\hbar\mathrm{d}/\mathrm{d}t = \mathrm{i}\hbar\partial/\partial t - \hbar\breve{L}$, where $\hbar\breve{L} := (\mathrm{d}Q/\mathrm{d}t)\breve{P} - (\mathrm{d}P/\mathrm{d}t)\breve{Q}$ is the *generalized Liouville operator*, and $\partial/\partial t := (\partial/\partial t)_{(Q,P)}$ denotes the time-rate of change at a fixed phase-space point (Q, P). This means that a stationary or *fixed observer* at the phase-space point (Q, P) finds that the rate of change of the state $|\psi(Q, P, t)\rangle$ is given by

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(Q, P, t)\rangle = (\hbar\breve{L} + \breve{\mathcal{D}})|\psi(Q, P, t)\rangle. \tag{10}$$

Consequently, a hypothetical *moving observer*, accompanying a phase-space image point $(Q(t), P(t))$, will at all times observe a non-vanishing rate of change of the quantum-mechanical state, as given by (8).

3. Extended classical dynamics

The objective of this section is to analyse the consequences of the equations (6) and (7) which we can think as defining a $\hbar$-dependent *extended classical dynamics*. Let us start by introducing the auxiliary quantities

$$V_\hbar(Q, P_0, t) := -\frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 S(Q, P_0, t)}{\partial Q^2} \qquad F_\hbar(Q, P_0, t) := -\frac{\partial V_\hbar(Q, P_0, t)}{\partial Q} \tag{11}$$

which, in virtue of the occurrence of the Planck constant $\hbar$ in (11), will be referred to as *quantum potential (energy)* and *quantum force*, respectively. Also note that $V(Q, t)$ and $V_\hbar(Q, P_0, t)$ play different roles in the theory, since the effective potential $V_\hbar(Q, P_0, t) + V(Q, t)$ is involved in (7), whereas in (6) only $V(Q, t)$ participates.

The term $V_\hbar(Q, P_0, t)$ in (7) arises from the quantum kinetic energy $\hat{p}^2/(2m)$, and its role seems analogous to that of the Bohmian quantum potential $V_R(x, t)$ in (3*a*). However, there are important differences between $V_\hbar(Q, P_0, t)$ and $V_R(x, t)$:

(i) $V_R(x, t)$ and its argument $x \in \Re^3$ are real-valued while, in contrast, $V_\hbar(Q, P_0, t)$ and its arguments Q and P_0 are in general complex-valued.

(ii) $V_R(x, t)$ is determined by the quantum state of the system, i.e. one has to solve first the Schrödinger equation to obtain the amplitude $R(x, t)$ of the wavefunction $\psi(x, t)$. In contrast, $V_\hbar(Q, P_0, t)$ is independent of the quantum state, except that P_0 depends on the initial quantum state at time t_0 (see equation (22)). It is worth mentioning here that $V_\hbar(Q, P_0, t)$ only can be determined after solving the QHJ equation (7) for $S(Q, P_0, t)$.

The QHJ equation (7) has the charm of being a $\hbar$-dependent stand-alone partial differential equation for $S(Q, P_0, t)$. Since it resembles the CHJ equation for an effective potential $V(Q, t) + V_\hbar(Q, P_0, t)$, one can interpret it as a classical equation that provides a way of adding quantum effects to classical dynamics. Let us now describe the method.

3.1. Link between P and $p(Q, P_0, t)$

As a general rule the GH equations (6) differ from the canonical Hamilton equations in that the first equation (6) includes on the right-hand side $p(Q, P_0, t)$ instead of P. To decode the relation between $p(Q, P_0, t)$ and P we apply the operator $\partial/\partial Q$ on equation (7) and use the definition of $p(Q, P_0, t)$, to obtain

$$\frac{\partial p}{\partial t} + \frac{p}{m}\frac{\partial p}{\partial Q} - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 p}{\partial Q^2} + \frac{\partial V}{\partial Q} = 0. \tag{12}$$

From this and (6), and the chain rule $\mathrm{d}p/\mathrm{d}t = \partial p/\partial t + (p/m)\partial p/\partial Q$, we get the relation

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -\frac{\partial V}{\partial Q} = \frac{\partial p}{\partial t} + \frac{p}{m}\frac{\partial p}{\partial Q} - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 p}{\partial Q^2} = \frac{\mathrm{d}p}{\mathrm{d}t} - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 p}{\partial Q^2}. \tag{13}$$

That is, the rate of change of the difference $(P - p)$ is given by

$$-\frac{\mathrm{d}}{\mathrm{d}t}(P - p) = F_\hbar(Q, P_0, t) := -\frac{\partial V_\hbar(Q, P_0, t)}{\partial Q} \tag{14}$$

which implies that

$$P(t) - p(Q(t), P_0, t) = \Lambda_0 - \int_{t_0}^{t} \mathrm{d}t' F_\hbar(Q(t'), P_0, t'). \tag{15}$$

Equation (15) introduces a new *parameter* defined by $\Lambda_0 := P_0 - p\,(Q_0, P_0, t_0)$, i.e. it measures the difference between the initial values of P_0 and $p\,(Q_0, P_0, t_0)$. Note that the quantum force vanishes in the particular case of quantum systems for which $S(Q, P_0, t)$ is a quadratic function of Q, namely $S(Q, P_0, t) = a_0(P_0, t) + a_1(P_0, t)Q + a_2(P_0, t)Q^2$.

3.2. Equivalence of (6) with Hamilton-like equations

After combining (6) and (14), we are able to rewrite the GH equations (6) in the form

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \frac{p}{m} \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial}{\partial Q}[V(Q, t) + V_\hbar(Q, P_0, t)] \tag{16}$$

with the initial condition $(Q_0, p(Q_0, P_0, t_0))$, and

$$p(Q_0, P_0, t_0) = P_0 - \Lambda_0 = \left.\frac{\partial S(Q, P_0, t_0)}{\partial Q}\right|_{Q=Q_0}. \tag{17}$$

That is, the extended classical dynamics is described by a set of Hamilton-like equations for a complex-valued and $\hbar$-dependent Hamiltonian $H_\hbar(Q, p, t) := p^2/(2m) + V(Q, t) + V_\hbar(Q, P_0, t)$, in which $V(Q, t)$ is augmented by the quantum potential $V_\hbar(Q, P_0, t)$. At this point, it is worth recalling that complex potentials, complex Hamiltonians and complex-valued trajectories play important roles in different fields of physics, e.g. [18–27].

Classical limit. In the limit $\hbar/m \to 0$ with $\partial^2 S(Q, P_0, t)/\partial Q^2$ kept finite, the quantum potential (11) vanishes and the set (16) reduces to the canonical Hamilton equations. The condition $\hbar/m \to 0$ means that the classical mechanics accurately describes the motion of the particle provided that $\hbar/m$ is small compared to a characteristic quantity of the system with dimensions of length^2/time, for example the product lv, where l is a typical distance over which the wavefunction changes significantly and v is a typical particle speed [28].

3.3. Link between (Q_0, P_0) and the initial wavefunction $\psi(x, t_0)$

Let us now demonstrate that the initial conditions for the Hamilton-like equation (16) are determined by the initial position-space wavefunction $\psi(x, t_0)$. For this, we withdraw the multi-index notation and rewrite (7) in a form similar to equation (3*a*):

$$\frac{\partial S(Q, P_0, t)}{\partial t} + \frac{1}{2m}[\nabla S(Q, P_0, t)]^2 - \frac{\mathrm{i}\hbar}{2m}\nabla^2 S(Q, P_0, t) + V(Q, t) = 0. \tag{18}$$

Since x is an argument of the position-space wavefunction $\psi(x, t)$, it is real-valued. Thus, in order to compare (18) and (3*a*) one must restrict considerations in (18) to real values of Q, i.e. $Q = x \in \Re^3$. In this case, one uses the decomposition $S(x, P_0, t) := A(x, P_0', P_0'', t) - \mathrm{i}\hbar B(x, P_0', P_0'', t)$, where A and B are real functions. By substituting this

into (18), and after separating real and imaginary parts, the following couple of real equations is obtained:

$$\frac{\partial A}{\partial t} + \frac{1}{2m}(\nabla A)^2 - \frac{\hbar^2}{2m}[\nabla^2 B + (\nabla B)^2] + V = 0 \tag{19a}$$

$$\frac{\partial B}{\partial t} + \frac{1}{m}(\nabla A)\cdot(\nabla B) + \frac{1}{2m}\nabla^2 A = 0. \tag{19b}$$

By comparing (19*a*) with (3*a*) we can identify the following quantities

$$A(x, P_0', P_0'', t) = \mathcal{W}(x, t) \tag{20a}$$

$$\nabla^2 B + (\nabla B)^2 = \frac{\nabla^2 R}{R} = \frac{\nabla^2 \rho^{1/2}}{\rho^{1/2}} = \frac{1}{2}\nabla^2 \ln \rho + \frac{1}{4}(\nabla \ln \rho)^2 \tag{20b}$$

and, therefore, $B(x, P_0', P_0'', t) = \frac{1}{2}\ln \rho(x, t)$. In addition, the vectorial identity $\nabla \cdot (\rho \boldsymbol{p}) = (\nabla \rho)\cdot \boldsymbol{p} + \rho(\nabla \cdot \boldsymbol{p})$, with $\boldsymbol{p} = \nabla \mathcal{W}$ allows us to demostrate that the equation (19*b*) is equivalent to continuity equation (3*b*).

In conclusion, on the *real axis* $Q = x \in \Re^3$ the solution $S(x, P_0, t)$ of the QHJ equation (18) is related to the position-space wavefunction $\psi(x, t)$ in the form

$$S(x, P_0, t) = \mathcal{W}(x, t) - \frac{\mathrm{i}\hbar}{2}\ln \rho(x, t). \tag{21}$$

Consequently, for $t = t_0$, equations (17) and (21) establish that the initial quantum state $\psi(x, t_0)$ fully determines the complex initial momentum $p(x_0, P_0, t_0)$ that corresponds to the *initial real coordinate* $Q_0 := Q(t_0) = x_0 \in \Re^3$, as given by

$$\begin{aligned} p(x_0, P_0, t_0) &= P_0 - \Lambda_0 \\ &= \left.\frac{\partial \mathcal{W}(x, t_0)}{\partial x}\right|_{x=x_0} - \left.\frac{\mathrm{i}\hbar}{2}\frac{\partial \rho(x, t_0)/\partial x}{\rho(x, t_0)}\right|_{x=x_0} := p_0' - \mathrm{i}p_0''. \end{aligned} \tag{22}$$

In concordance with the considerations of the appendix, the parameter $\Lambda_0 := P_0 - p(Q_0, P_0, t_0)$ is hereafter fixed as $\Lambda_0 = 0$. As a result, $P_0 = P_0' + \mathrm{i}P_0''$ is a complex-valued quantity, with $P_0' := p_0'$ and $P_0'' := -p_0''$.

At this point, some comments on the effects of the quantum potential within the extended classical dynamics are in order:

(i) Consider a phase-space trajectory with initial condition $(x_0, p_0' - \mathrm{i}p_0'')$. If the complex-valued quantum potential $V_\hbar(Q, P_0, t)$ were absent in (16) (i.e. in the classical limit when $\hbar/m \to 0$), this trajectory would be equivalent to two *uncoupled* phase-space trajectories with initial conditions (x_0, p_0') and $(x_0, -p_0'')$. However, since $V_\hbar(Q, P_0, t)$ does exist in (16), the initial condition $(x_0, p_0' - \mathrm{i}p_0'')$ and the equations (16) lead to a new single complex-valued phase-space trajectory, which cannot be constructed from the uncoupled real-valued trajectories (x_0, p_0') and $(x_0, -p_0'')$.

(ii) Consider a complex-valued initial state $\psi(x, t_0)$ in the polar form (2), and recall (22), and the expression $\rho(x, t_0) = |\psi(x, t_0)|^2 \geqslant 0$. At the critical points of $\rho(x, t_0)$, in particular at the nodes of the initial state $\psi(x, t_0)$, the initial momentum P_0 is a purely real number, whereas it is a purely imaginary number at the critical points of $\mathcal{W}(x, t_0)$. Thus, the sets of critical points of $\rho(x, t_0)$ and $\mathcal{W}(x, t_0)$ play a privileged role in the extended classical dynamics. In fact, by selecting a critical point x_0 and fixing the corresponding initial condition, either (x_0, p_0') or $(x_0, -p_0'')$, a phase-space trajectory is generated by the

equations (16). However, since the initial condition is real-valued, the effects of the kind (i) are absent and so the trajectory only undergoes the effects due to the effective potential $V(Q,t) + V_\hbar(Q, P_0, t)$.

(iii) A similar behaviour to (ii) exists in the case of a real-valued initial state $\psi(x, t_0)$, because the initial conditions for (16) are then of the form $(x_0, -p_0'')$.

4. Phase-space quantum dynamics

In this section our task is mainly to consider the quantum dynamics as described by equations (8) and (10), and to introduce the so-called semiclassical approximation as stated in the contents.

The phase-space wavefunction of the quantum state (5) is given by the scalar product $\psi(Q, P, t) := \langle 0|\psi(Q, P, t)\rangle$, where $|0\rangle := |Z = 0\rangle$ is the coherent state $|Z = 0\rangle$, i.e. the ground state of the f-dimensional harmonic oscillator (in the present paper, $f = 3$). The wavefunction $\psi(Q, P, t)$ satisfies equations of motion that are identical in form to (8) and (10). On the other hand, the position and momentum wavefunctions can be obtained from $\psi(Q, P, t)$, when $Q = Q' + \mathrm{i}Q''$ and $P = P' + \mathrm{i}P''$ are complex-valued parameters, by using relations (67) and (70) of [17], in the form:

$$\psi(Q', t) = (2\sqrt{\pi}\, p_o)^{-f/2}(2\pi\hbar)^{-f/2}\int_{-\infty}^{\infty} \mathrm{d}P' \exp\left(\frac{\mathrm{i}}{\hbar}S(Q', P_0, t)\right)\psi(Q', P' + \mathrm{i}P'', t) \qquad (23)$$

and

$$\tilde{\psi}(P', t) = (2\sqrt{\pi}q_o)^{-f/2}(2\pi\hbar)^{-f/2} \times \int_{-\infty}^{\infty} \mathrm{d}Q' \exp\left(-\frac{\mathrm{i}}{\hbar}QP'\right)\exp\left(\frac{\mathrm{i}}{\hbar}S(Q, P_0, t)\right)\psi(Q, P', t) \qquad (24)$$

where q_o and p_o are position and momentum units restricted by the condition $q_o p_o = \hbar$. Here we are using the notation $Q = (Q_1, Q_2, Q_3) = Q' + \mathrm{i}Q''$, with $Q' = (Q_1', Q_2', Q_3')$ and $\mathrm{d}Q' = \mathrm{d}Q_1'\,\mathrm{d}Q_2'\,\mathrm{d}Q_3'$, and so on. That is $Q' \in \Re^3$ and $P' \in \Re^3$ are real-valued quantities.

Let us stress that the only role of the factor $\exp(\mathrm{i}S(Q, P_0, t)/\hbar)$ entering the integrands of (23) and (24) is to *counterbalance* the factor $\exp(-\mathrm{i}S(Q, P_0, t)/\hbar)$ included in the definition of the phase-space wavefunction $\psi(Q, P, t)$.

4.1. Semiclassical approximation

The semiclassical approximation is defined as the one characterized by neglecting in (10) the effects due to the phase-space operator $\breve{\mathcal{D}}$, i.e. by taking into account only the *Liouvillian flow* due to the operator $\breve{L}$. In this approximation, $\psi(Q, P, t)$ is *fully* transported in the complex phase space by the ensemble of classical trajectories, obtained as the solutions to (6). That is,

$$\psi_{scl}(Q, P, t) = \psi(Q_0(Q, P, t), P_0(Q, P, t), t_0) \qquad (25)$$

where $(Q(t), P(t))$ is the trajectory passing through the point $(Q_0, P_0) := (Q(t_0), P(t_0))$ at time t_0. Since the flow generated by the extended classical dynamics is generally $\hbar$-dependent, the semiclassical approximation (25) could give not only a simplified picture of the quantum time evolution but also a more useful one.

4.2. The image arising from the phase-space picture

At this point, a conceptual comparison with the interaction picture can help for grasping the physical meaning of the phase-space picture. The interaction picture transforms the

Schrödinger equation for the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}(t)$ with the goal of separating the free motion due to $\hat{H}_0$ from the motion of the total system, so that the resulting state vector is time-dependent, but this dependence is entirely due to the interaction $\hat{V}(t)$.

In the case of the phase-space picture of the QM, the physical goal is to decompose the quantum effects into two groups: (i) the contribution of the Liouvillian flow (operator $\breve{L}$) that leads up to the semiclassical aproximation (25). In this approximation, the $\hbar$-dependent extended classical dynamics is enough to describe the evolution of the quantum state $\psi(Q, P, t)$ in the phase space; (ii) the effects stemming from the phase operator $\breve{\mathcal{D}}$, which take care of higher-order quantum effects in $\hbar$.

4.3. Contrast between Bohmian, Wigner and phase-space trajectories

Let us emphasize that the Bohmian trajectories are the basis for the Bohmian mechanics [1, 2, 5], whereas the present phase-space trajectories are only a tool for solving the Schrödinger equation. In this sense, they resemble the Wigner trajectories [11, 29]. This concept and its limitations have been discussed in [29], where it was also found that under certain circumstances a process of creation and destruction of Wigner trajectories exists. Consequently, the applicability of such a concept is limited.

It seems that the phase-space trajectories proposed in the present paper are not destroyed or created by virtue of two facts: (i) they are complex-valued and independent of the quantum state, with the exception that the initial quantum state $\psi(x, t_0)$ fixes the initial conditions for the ensemble of trajectories (see equation (22)); (ii) they have as the classic limit ($\hbar/m \to 0$) the classical trajectories given by the canonical Hamilton equations, which is a sound property for developing semiclassical approximations [29].

5. One-dimensional driven harmonic oscillator

This section has two goals: (i) illustrate the phase-space technique described in this paper by applying it to the one-dimensional driven oscillator, and (ii) generate a complete orthonormal set of functions $\{\psi_n(Q, P, t), n = 0, 1, 2, \ldots\}$, i.e. a basis for future quantum-mechanical calculations in the phase space.

We consider a Hamiltonian $H(\hat{q}, \hat{p}, t) = H_0(\hat{q}, \hat{p}) - F(t)\hat{q}$, where $H_0(\hat{q}, \hat{p}) = \hat{p}^2/(2m) + \left(m\omega_0^2/2\right)\hat{q}^2$ describes a one-dimensional harmonic oscillator of mass m and frequency ω_0, and $F(t)$ is a real function of time t corresponding to a spatially uniform force.

5.1. Solution of the quantum Hamilton–Jacobi equation

The QHJ equation (7) becomes

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial Q}\right)^2 - \frac{\mathrm{i}\hbar}{2m}\frac{\partial^2 S}{\partial Q^2} + \frac{1}{2}m\omega_0^2 Q^2 - F(t)Q = 0 \qquad S(Q, P_0, t_0) = P_0 Q. \tag{26}$$

Equation (26) for $S(Q, P_0, t)$ can be solved by using the ansatz

$$S(Q, P_0, t) = -s(t, t_0) + y(t, t_0)Q - \tfrac{1}{2}m\Omega(t, t_0)Q^2 \tag{27}$$

which leads to $\mathrm{d}\Omega/\mathrm{d}t = \Omega^2 + \omega_0^2$, $\mathrm{d}y/\mathrm{d}t = \Omega y + F(t)$ and $\mathrm{d}s(t)/\mathrm{d}t = (y^2 + \mathrm{i}\hbar m\Omega)/(2m)$. After integrating these equations and by introducing the definition $\delta_0 := -\omega_0 t_0$, we obtain

$$\Omega(t, t_0) = \omega_0 \tan(\omega_0 t + \delta_0) \qquad y(t, t_0) = \frac{P_0 + \beta(t, t_0)}{\cos(\omega_0 t + \delta_0)}$$

$$\begin{aligned} s(t, t_0) &= \frac{1}{2m}\int_{t_0}^{t} \mathrm{d}t' y^2(t') - \frac{\mathrm{i}\hbar}{2}\ln(\cos(\omega_0 t + \delta_0)) \\ &= \frac{P_0^2}{2m}\Delta_0(t, t_0) + \frac{P_0}{m}\Delta_1(t, t_0) + \frac{1}{2m}\Delta_2(t, t_0) - \frac{\mathrm{i}\hbar}{2}\ln(\cos(\omega_0 t + \delta_0)) \end{aligned} \tag{28}$$

with the auxiliary quantities

$$\begin{aligned} \beta(t, t_0) &:= \int_{t_0}^{t} \mathrm{d}t' F(t')\cos(\omega_0 t' + \delta_0) \\ \alpha(t, t_0) &:= -\frac{1}{m\omega_0}\int_{t_0}^{t} \mathrm{d}t' F(t')\sin(\omega_0 t' + \delta_0) \\ \gamma(t, t_0) &:= \frac{1}{2m\omega_0}\int_{t_0}^{t} \mathrm{d}t'' \int_{t_0}^{t''} \mathrm{d}t' F(t'')F(t')\sin(\omega_0(t'' - t')) \\ \Delta_n(t, t_0) &:= \int_{t_0}^{t} \mathrm{d}t' \frac{\beta^n(t', t_0)}{\cos^2(\omega_0 t' + \delta_0)} \qquad \text{where} \quad n = 0, 1, 2. \end{aligned} \tag{29}$$

Note that integration by parts gives the relations $\Delta_0(t, t_0) = \tan(\omega_0 t + \delta_0)/\omega_0$, $\Delta_1(t, t_0) = m\alpha(t, t_0) + \beta(t, t_0)\Delta_0(t, t_0)$ and $\Delta_2(t, t_0) = \beta(t, t_0)\Delta_1(t, t_0) - 2m\gamma(t, t_0)$.

5.2. Solution of the generalized Hamilton equations

From (27), (11) and (15), we obtain the quantum potential $V_\hbar(Q, P_0, t) = (\mathrm{i}\hbar/2)\Omega(t)$, the quantum force $F_\hbar(Q, P_0, t) = 0$ and the relation $P(t) = p(Q(t), P_0, t)$. Thus the Hamilton-like equations (16) become $\mathrm{d}Q/\mathrm{d}t = P/m$ and $\mathrm{d}P/\mathrm{d}t = -m\omega_0^2 Q + F(t)$, with the initial condition (Q_0, P_0). The solution is given by

$$\begin{bmatrix} Q(t) \\ P(t) \end{bmatrix} = \begin{bmatrix} \cos(\omega_0 t + \delta_0) & \sin(\omega_0 t + \delta_0)/(m\omega_0) \\ -m\omega_0 \sin(\omega_0 t + \delta_0) & \cos(\omega_0 t + \delta_0) \end{bmatrix} \begin{bmatrix} Q_0 + \alpha(t, t_0) \\ P_0 + \beta(t, t_0) \end{bmatrix}. \tag{30}$$

The points $(Q(t_0), P_0)$ and $(Q(t), P(t))$ belong to the same phase-space trajectory, and they are connected by (30) or, equivalently, by the inverse transformation,

$$\begin{bmatrix} Q_0 \\ P_0 \end{bmatrix} = \begin{bmatrix} \cos(\omega_0 t + \delta_0) & -\sin(\omega_0 t + \delta_0)/(m\omega_0) \\ m\omega_0 \sin(\omega_0 t + \delta_0) & \cos(\omega_0 t + \delta_0) \end{bmatrix} \begin{bmatrix} Q(t) - a(t, t_0) \\ P(t) - b(t, t_0) \end{bmatrix} \tag{31}$$

with the auxiliary quantities

$$\begin{bmatrix} a(t, t_0) \\ b(t, t_0) \end{bmatrix} := \begin{bmatrix} \cos(\omega_0 t + \delta_0) & \sin(\omega_0 t + \delta_0)/(m\omega_0) \\ -m\omega_0 \sin(\omega_0 t + \delta_0) & \cos(\omega_0 t + \delta_0) \end{bmatrix} \begin{bmatrix} \alpha(t, t_0) \\ \beta(t, t_0) \end{bmatrix}. \tag{32}$$

Let us note that $a(t, t_0)$ satisfies the equation of motion $m\ddot{a} = -m\omega_0^2 a + F(t)$, $b(t, t_0) = m\dot{a}(t, t_0)$, and that the quantities $\alpha(t, t_0)$, $\beta(t, t_0)$, $a(t, t_0)$ and $b(t, t_0)$ have their origin in the force $F(t)$. In comparison with the unperturbed harmonic oscillator the net result of $F(t)$ is to shift either the initial state (Q_0, P_0) or the end state (Q, P).

Differing from classical mechanics, the solution (30) of the Hamilton-like equations allows for complex values of Q and P, because P_0 is generally complex-valued. In addition, since (30) is a linear transformation connecting the states (Q_0, P_0) and (Q, P), then a complex trajectory $(Q(t), P(t)) = (Q'(t) + \mathrm{i}Q''(t), P'(t) + \mathrm{i}P''(t))$ may be viewed as the combination of two real-valued solutions of the Hamilton equations, namely $(Q'(t), P'(t))$ and $(Q''(t), P''(t))$.

5.3. Evolution of the quantum state

Let us consider the time evolution of the system as seen by a *fixed observer* at the point (Q, P), who has to solve the Schrödinger equation (10) with the phase-space operators

$$\hbar\breve{L} = \frac{P}{m}\breve{P} + \left(m\omega_0^2 Q - F(t)\right)\breve{Q} \qquad \breve{\mathcal{D}} = \frac{1}{2m}\breve{P}^2 + \frac{1}{2}m\omega_0^2\breve{Q}^2. \tag{33}$$

For solving (10) one takes advantage of the interaction picture for getting the exact solution $|\psi(t)\rangle$, and afterwards the initial state is fixed as $|\psi(t_0)\rangle = |n\rangle$, where $|n\rangle$ is an energy eigenstate of the unperturbed harmonic oscillator.

Let us recall the auxiliary functions [17]

$$M(Q) := (\sqrt{\pi q_o})^{-f/2}\exp[-(\kappa_o Q)^2] \tag{34}$$

$$\tilde{M}(P) := (\sqrt{\pi}\, p_o)^{-f/2}\exp[-(\chi_o P)^2] \tag{35}$$

where $\kappa_o := (\sqrt{2}q_o)^{-1}$ and $\chi_o := (\sqrt{2}p_o)^{-1}$. By using (55b) of [17] we obtain the phase-space wavefunction

$$\begin{aligned}\psi_n(Q, P, t) = {} & \exp\left(\frac{\mathrm{i}}{\hbar}\gamma\right)\exp\left(-\frac{\mathrm{i}}{\hbar}S(Q, P_0, t)\right)\exp\left(\frac{\mathrm{i}}{2\hbar}[QP + \beta Q_0 - \alpha P_0]\right)\\ & \times\exp\left(-\frac{\mathrm{i}\omega_0}{2}(t - t_0)\right)[(\pi\hbar)^{1/2}M(Q_0)\tilde{M}(P_0)]^{1/2}\frac{1}{\sqrt{n!}}[\kappa_o Q_0 - \mathrm{i}\chi_o P_0]^n\end{aligned} \tag{36}$$

where the points (Q_0, P_0) and (Q, P) are related by the transformation (31). Equivalently, the wavefunction $\psi_n(Q, P, t)$ can be expressed in the form

$$\begin{aligned}\psi_n(Q, P, t) = {} & \exp\left(\frac{\mathrm{i}}{\hbar}\gamma\right)\exp\left(-\frac{\mathrm{i}}{\hbar}S(Q, P_0, t)\right)\exp\left(\frac{\mathrm{i}}{2\hbar}[QP + bQ - aP]\right)\\ & \times\exp\left(-\mathrm{i}\omega_0\left(n + \frac{1}{2}\right)(t - t_0)\right)[(\pi\hbar)^{1/2}M(Q - a)\tilde{M}(P - b)]^{1/2}\\ & \times\frac{1}{\sqrt{n!}}[\kappa_o(Q - a) - \mathrm{i}\chi_o(P - b)]^n.\end{aligned} \tag{37}$$

In the above equations the arguments of $\alpha(t, t_0)$ and other quantities are suppressed.

5.4. Position and momentum wavefunctions

In this section, our task is to determine the position-space wavefunction $\psi(Q', t)$ by applying the relation (23) to the phase-space wavefunction (37). After the replacement $Q \to Q' \in \Re$, by expanding $[\kappa_o(Q' - a) - \mathrm{i}\chi_o(P - b)]^n$, recalling that $P = P' + \mathrm{i}P''$ is complex-valued, and using the Rodrigues formula and the identity [30]

$$\sum_{k=0}^{n}\binom{n}{k}(2y)^{n-k}H_k(x) = H_n(x + y) \tag{38}$$

we obtain that the wavefunction in position space is given by

$$\begin{aligned}\psi_n(Q', t) = {} & \exp\left(\frac{\mathrm{i}}{\hbar}\gamma\right)\exp\left(-\mathrm{i}\omega_0\left(n + \frac{1}{2}\right)(t - t_0)\right)\exp\left(\frac{\mathrm{i}}{\hbar}\left(Q' - \frac{a}{2}\right)b\right)\\ & \times\frac{1}{\sqrt{2^n n!}}M(Q' - a)H_n\left(\frac{Q' - a}{q_o}\right).\end{aligned} \tag{39}$$

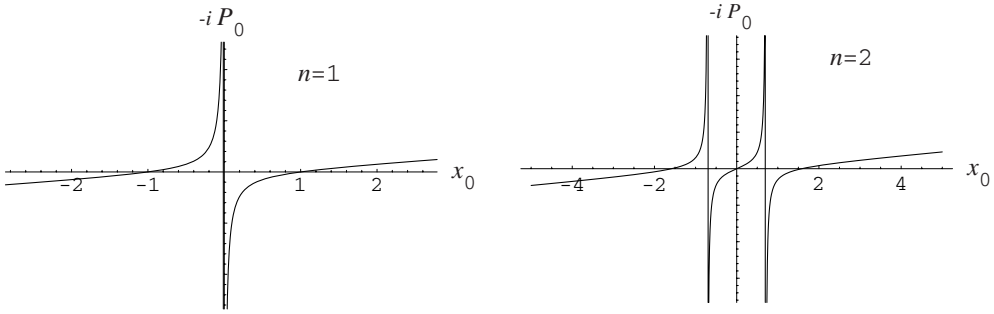

Figure 1. In accordance with (41), the behaviour of P_0 as a function of the initial position $Q_0 = x_0 \in \Re$ is determined by the zeros of the Hermite polynomials. For the ground state ($n = 0$) the relation is linear, $P_0 = \mathrm{i}(p_o/q_o)x_0$.

A similar procedure allows us to determine the wavefunction $\tilde{\psi}(P', t)$ in momentum space by applying the relation (24) to the phase-space wavefunction (37). The result is

$$\tilde{\psi}(P', t) = \exp\left(\frac{\mathrm{i}}{\hbar}\gamma\right)\exp\left(-\mathrm{i}\omega_0\left(n+\frac{1}{2}\right)(t-t_0)\right)\exp\left(-\frac{\mathrm{i}}{\hbar}a\left(P'-\frac{b}{2}\right)\right)$$
$$\times\frac{(-\mathrm{i})^n}{\sqrt{2^n n!}}\tilde{M}(P'-b)H_n\left(\frac{P'-b}{p_o}\right). \tag{40}$$

5.5. Image of the moving observer

Let us now consider the time evolution of the system as seen by a *moving observer* travelling in phase space with the point $(Q(t), P(t))$, who has to solve the Schrödinger equation (8). The descriptions of the fixed observer and the moving observer are physically equivalent, provided that the solution of (8) is obtained from (36), or from (37), by doing the substitutions $Q \to Q(t)$ and $P \to P(t)$, where $Q(t)$ and $P(t)$ are related to the initial state (Q_0, P_0) by the equation (30).

In order to apply (30), we must set up the initial condition (Q_0, P_0) for each trajectory. To do this we consider that at t_0 the *initial position wavefunction* is $\psi(x_0, t_0) = \varphi_n(x_0) := \langle x_0 \,|n\rangle$, i.e. the nth eigenfunction of the harmonic oscillator. Since $\varphi_n(x_0)$ is real, then $\mathcal{W}(x_0, t_0) = 0$, and the initial probability density is given by $\rho(x_0, t_0) = \varphi_n^2(x_0)$. Therefore, for a given initial position $x_0 \in \Re$, equation (22) and the relation $(\mathrm{d}/\mathrm{d}x)H_n(x) = 2nH_{n-1}(x)$ give the initial momentum

$$P_0(x_0) = \mathrm{i}p_o\left[\frac{x_0}{q_o} - \sqrt{2n}\frac{\varphi_{n-1}(x_0)}{\varphi_n(x_0)}\right] = \mathrm{i}p_o\left[\frac{x_0}{q_o} - 2n\frac{H_{n-1}(x_0/q_o)}{H_n(x_0/q_o)}\right] := \mathrm{i}P_0'' \tag{41}$$

with $\varphi_{-1}(x_0, t_0) := 0$ and $H_{-1}(x) := 0$. If the initial state is the ground state $n = 0$, then $P_0 = \mathrm{i}(p_o/q_o)x_0$. In the general case (see figure 1), since P_0 has poles at all n real zeros of the Hermite polynomial $H_n(x_0/q_o)$, $-\mathrm{i}P_0$ is an increasing function of x_0 between two successive zeros of $H_n(x_0/q_o)$.

6. Concluding remarks

Let us now sum up other points emerging in this work for the general case of a particle with potential energy $V(Q, t)$:

(i) Since the Schrödinger equation (10) and the corresponding equation for $\psi(Q, P, t) := \langle 0|\psi(Q, P, t)\rangle$ are lineal, the probability amplitude $\psi(Q, P, t)$ obeys the superposition principle. Thus, $\psi(Q, P, t)$ can be expanded in terms of a basis $\{\psi_n(Q, P, t)\}$, for example the one constructed with elements given by (36) or (37). In practice, a truncation procedure is applied and only a finite set of coefficients $\{c_n(t), n = 0, 1, 2, \ldots, N\}$ is obtained.

(ii) After having the set of N coefficients $c_n(t)$, an approximation of the phase-space wavefunction $\psi(Q, P, t)$ may be used, and approximate position and momentum wavefunctions can be calculated from (23) and (24). However, for counterbalancing the factor $\exp(\mathrm{i}S(Q, P_0, t)/\hbar)$ entering the integrands, first the QHJ equation (7) has to be solved for $S(Q, P_0, t)$. This function is also required for setting the Hamiltonian $H_\hbar(Q, p, t)$ involved in the Hamilton-like equations (16).

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Appendix

Reasons for choosing the parameter $\Lambda_0 := P_0 - p(Q_0, P_0, t_0)$ as $\Lambda_0 = 0$.

Let us begin with equation (22), and consider three particular choices of the parameter Λ_0: (i) $\Lambda_0 = 0$, $P_0 = p(Q_0, P_0, t_0)$, (ii) $P_0 = p_0'$, $\Lambda_0 = \mathrm{i}p_0''$ and (iii) $P_0 = -\mathrm{i}p_0''$, $\Lambda_0 = -p_0'$. These selections are physically equivalent because the initial conditions for the equations (7) and (16) only depend on Q_0 and $p(Q_0, P_0, t_0)$. However, the choice (ii) and the Hamilton equations (16) only give information about the time evolution of the real part of (22), similarly (iii) only evolves the pure imaginary part of (22), whereas (i) considers the *whole initial state* (22). Thus, the choice (i) appears to be the best option, and therefore $\Lambda_0 = 0$.

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