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The quantum motion of half-densities and the derivation of Schrödinger's equation

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Abstract. The notion of half-density has been used for a long time within the context of the semiclassical approximation. We show in this paper that the inclusion of half-densities in Bohmian mechanics leads to a very simple theory of motion when one uses Hamilton–Jacobi theory; in particular, one immediately recovers Maslov's semiclassical approximation without extra calculations.

1. Introduction

The mathematical foundations of Bohmian mechanics, also known as ‘the quantum theory of motion’ [13], have recently received much attention; Berndl *et al* [2] have, for instance, proven global existence theorems for large classes of potentials; in Dürr *et al* [4] one finds an analysis of the conceptual principles of Bohmian mechanics. Also see Holland's treatise [13] for a careful analysis of Hamilton–Jacobi theory within the context of Bohmian mechanics. The aim of this paper is to relate Bohmian mechanics to the theory of half-densities on Lagrangian manifolds which we introduced in de Gosson [10, 11]. The underlying idea is that it is the square roots of densities, and not the densities themselves, which intervene in quantum mechanics. This idea is certainly not new, and can be traced back to van Vleck [20]. It is being used in various quantization schemes related to semiclassical approximation theories (for instance, the WKB method) together with the ‘metaplectic correction’, where it is fruitfully used to eliminate the difficulties due to the occurrence of ‘caustics’; see, for instance, [9] and the references therein. Surprisingly enough, it turns out that the inclusion of half-densities in Bohmian mechanics leads to a quantum mechanics in phase space totally different from the traditional Wigner–Weyl–Moyal formalism or its variants. We are actually going to show (proposition 2, section 3) that if one transports an ‘initial’ half-density $\Psi_0(q)|d^n q|^{1/2}$ using the Hamiltonian flow associated to the ‘Bohmian’ $H + U^\psi$ (U^ψ the ‘quantum potential’) then one obtains, up to a phase factor \aleph , the half-density $(Q, t)|d^n Q|^{1/2}$ where Q is the point of the trajectory originating from q at time $t = 0$ and reached at time t , and $\psi(\cdot, t)$ is the solution to Schrödinger's equation associated with H and such that $\psi(\cdot, 0) = \psi_0$. The phase factor is then the exponential

$$\aleph = \exp \left[\frac{i}{\hbar} \int p \, dq - (H + U^\psi) \, dt \right]$$

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where the action integral is calculated along the Bohmian trajectory in phase space starting from the point $(q, \nabla_q S_0(q))$ at the instant $t = 0$ and reaching the point $(Q, \nabla_Q S_0(Q, t))$ at time t . That Bohmian trajectory is determined by the usual Hamilton equations of motion, associated not to the Hamiltonian H , but to the ‘Bohmian’ $H + U^\psi$. If one neglects the quantum potential U^ψ , then one recovers the usual formulae of the semiclassical approximation, as in, for instance, Maslov and Fedoriuk [16]. This is conceptually interesting, because it clearly demonstrates that the domain of validity of the semiclassical approximation is that of vanishing quantum potentials, and that the Bohmian theory of motion allows the use of concepts and terminology from classical mechanics to study quantum mechanics.

We begin by showing in section 2 that Schrödinger’s equation for quadratic Hamiltonians can be derived from classical mechanics using equation (2.10) which governs the evolution of the square root of a density.

2. Derivation of Schrödinger’s equation for quadratic Hamiltonians

It is a well known fact that Schrödinger’s equation can be derived from Hamilton’s equations of motion for all polynomial Hamiltonians that are at most quadratic functions of the coordinates q, p ([6, 9, 12, 18] is certainly a non-exhaustive list of references where this is explicitly done). The usual argument goes as follows: the flow $(f_t)_t$ associated with such a Hamiltonian consists of *linear* symplectic transforms, and can thus be ‘lifted’ to a group $(F_t)_t$ of unitary operators acting on $L^2(\mathbb{R}_q^n)$ (in fact, a subgroup of the metaplectic group $Mp(n)$, which is a twofold covering group of the symplectic group $Sp(n)$). One then checks, using a Lie algebra argument (see [6–8, 12, 14, 15]) that $(F_t)_t$ satisfies Schrödinger’s equation

$$i\hbar \frac{d}{dt} F_t = \hat{H} F_t \quad (2.1)$$

where \hat{H} is the usual Hamiltonian operator associated with H . We are going to give in this section a *direct* derivation of Schrödinger’s equation for all Hamiltonians of the type

$$H(q, p, t) = \frac{1}{2} p^2 + \frac{1}{2} Rq \cdot q \quad (2.2)$$

where R is a real symmetric $n \times n$ matrix; we are using here obvious notation, for instance we have set $p^2 = p_1^2 + \dots + p_n^2$. The argument that will follow can actually be adapted with some minor modifications to arbitrary quadratic Hamiltonians with time-dependent coefficients. It is a variant of that used in [18] and involves less calculations. It demonstrates, moreover, our aim clearly, which is to advertise the essential role played by the notion of half-density in the context of Schrödinger’s equation. We first observe that Hamilton’s equations of motion for H are

$$\frac{dq}{dt} = p \quad \frac{dp}{dt} = -Rq \quad (2.3)$$

so that the Hamiltonian flow $(f_t)_t$ is a one-parameter subgroup of the symplectic group $Sp(n)$; in fact,

$$f_t = \exp \left[t \begin{pmatrix} 0 & tI \\ -R & 0 \end{pmatrix} \right] \quad (2.4)$$

so that for small values of $|t|$ we have

$$f_t = \begin{pmatrix} 0 & tI \\ -tR & 0 \end{pmatrix} + \mathcal{O}(t^2). \quad (2.5)$$

Here I (respectively, 0) is the $n \times n$ identity (respectively, zero) matrix and $O(t^2)$ is a $2n \times 2n$ matrix whose entries are all $O(t^2)$. It follows that there exists $T > 0$ such that f_t is a free symplectic transformation for $0 < |t| < T$. Now let S be the two-point free generating function determined by H (see, for instance, [1]). This function is determined by the conditions

$$(Q, P) = f_t(q, p) \Leftrightarrow \begin{cases} P = \frac{\partial S}{\partial Q}(Q, q, t) \\ p = -\frac{\partial S}{\partial q}(Q, q, t) \end{cases} \tag{2.6}$$

and satisfies the relation

$$S(q(t), q, t) = \int_0^t p \, dq - H \, dt' \tag{2.7}$$

where the integral is calculated along the trajectory from q to $Q = q(t)$. It follows from (2.7) that S satisfies the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + H(Q, \nabla_Q S) = 0. \tag{2.8}$$

Another important property of S is the following: denote by $J(Q, q, t)$ the determinant of the Hessian (matrix of second derivatives) of $S(Q, q, t)$:

$$J(Q, q, t) = \det \frac{\partial^2 S}{\partial Q \partial q}(Q, q, t). \tag{2.9}$$

Then J satisfies the ‘continuity equation’.

$$\frac{\partial J}{\partial t} + \nabla_Q \cdot J \nabla_p H = 0. \tag{2.10}$$

(See [16, lemma 3.2.1, p 96]). This property in fact holds true for the free generating function determined by an arbitrary Hamiltonian. However, in the present case (quadratic Hamiltonian) the f_t are linear, and the generating function S is thus itself quadratic in the variables Q and q , as can easily be seen from (2.4) and (2.7), so that J does not contain the variables q and Q . Equation (2.10) thus becomes

$$\frac{\partial J}{\partial t} + J \nabla_Q^2 S = 0 \tag{2.11}$$

noting that $\nabla_p H = \nabla_Q S$ in view of (2.3) and (2.6). Let now ψ_0 be an ‘initial wavefunction’; we assume that ψ_0 is in the Schwartz space $\mathcal{S}(\mathbb{R}_q^n)$, but the argument we are going to present obviously remains valid under less stringent conditions on ψ_0 . We claim that a solution to Schrödinger’s equation

$$i\hbar \frac{d\psi}{dt} = H(q, -i\hbar \nabla_q) \psi \tag{2.12}$$

is given, for $0 < |t| < T$, by the formula

$$\psi(q, t) = (2\psi i\hbar)^{-n/2} a(t) \int \exp\left(\frac{i}{\hbar} S(q, q', t)\right) \psi_0(q') \, d^n q' \tag{2.13}$$

where $a(t)$ is a conveniently chosen ‘square root’ of $J(t)$. In fact, that square root can be chosen in such a way that

$$\lim_{t \rightarrow 0} \Psi(q, t) = \Psi_0(q). \tag{2.14}$$

The proof goes as follows. Differentiating both sides of (2.13) with respect to the variable t and taking the Hamilton–Jacobi equation (2.8) into account, we get

$$i\hbar \frac{\partial \psi}{\partial t} = (2\pi i\hbar)^{-n/2} \int \exp\left(\frac{i}{\hbar} S\right) \left[H(q, -i\hbar \nabla_q a) + i\hbar \frac{\partial a}{\partial t} \right] \psi_0(q') d^n q'.$$

Performing similar calculations for the second-order q -derivatives we also have

$$H(q, -i\hbar \nabla_q) \psi = (2\pi i\hbar)^{-n/2} \int \exp\left(\frac{i}{\hbar} S\right) \left[H(q, -i\hbar \nabla_q a) + \frac{1}{2} a \nabla_q^2 S \right] \psi_0(q') d^n q'.$$

Now, $a = \sqrt{J}$ satisfies the equation

$$\frac{\partial a}{\partial t} + \frac{1}{2} \nabla_q^2 S \cdot a = 0 \quad (2.15)$$

in view of (2.10) and ψ thus solves Schrödinger’s equation (2.12) as claimed. Suppose now we let $t \rightarrow 0+$; we can evaluate the integral on the right-hand side of (2.12) by the method of the stationary phase, and one finds that $\lim_{t \rightarrow 0} \Psi(q, t) = \pm \Psi_0(q)$, depending on how the argument of the square root of J is chosen: if $J(t) > 0$ then $\sqrt{J(t)} = \pm (J(t))^{1/2}$, if $J(t) < 0$ then $\sqrt{J(t)} = \pm i |J(t)|^{1/2}$. It turns out that there exists efficient and systematic procedures for determining the correct choice; they suggest to us the notion of *Maslov index* which we have extensively analysed in [6–8]. If, for instance, we write f_t in block-matrix form

$$f_t = \begin{pmatrix} A(t) & B(t) \\ C(t) & D(t) \end{pmatrix}$$

then a straightforward calculation involving (2.6) yields

$$S(q, q', t) = \frac{1}{2} D B^{-1} q \cdot q - B^{-1} q \cdot q' + \frac{1}{2} B^{-1} A q' \cdot q' \quad (2.16)$$

and

$$\psi(q, t) = \left(\frac{1}{2\pi i\hbar} \right)^{n/2} i^{m(t)} |\det(B(t))|^{-1/2} \int e^{(i/\hbar) S(q, q', t)} \psi_0(q') dq' \quad (2.17)$$

where $m(t)$ is the inertia (= number of less than zero eigenvalues) of the matrix $B(t)$; one thus recovers the Robbin–Salamon formula (theorem 8.5 in [17]). We shall not continue to discuss these formalities here, because what is really important for our present purpose is that we used, to derive Schrödinger’s equation (2.12), the only Hamilton–Jacobi equation (2.8) together with equation (2.14) which governs the evolution of the *square root* of a density, i.e. of a *half-density*. We notice that explicit formulae of the type (2.17) are often used in the physical literature, the usual reference being Feynman–Hibbs [4]. We want, however, to emphasize that this formula is not obtained by dubious ‘path integral’ techniques, but is a simple rigorous consequence of classical Hamilton–Jacobi theory as we have just shown. We also observe that from classical mechanics we cannot claim that we have derived *quantum mechanics*: we have only derived Schrödinger’s equation. For quantum mechanics to become effective one needs to justify the need for Planck’s constant \hbar . This is particularly apparent for Hamiltonians of the type considered in this section, because of Ehrenfest’s theorem on average values. For instance, if one imposes that the initial wavefunction Ψ_0 is a Gaussian ‘minimum wavepacket’, then the evolution of $|\Psi(q, t)|^2$ and of $|\Phi(p, t)|^2$ (Φ the Fourier transform of Ψ) is that of classical Gaussian probability densities with spreading $\Delta q(t)$ and $\Delta p(t)$ such that $\Delta p(t) \Delta q(t) \geq \hbar/2$ and this is true for *any* value of \hbar . For a discussion of the need for Planck’s constant, and an effective quantization procedure making use of the Maslov index and leading in a rigorous way to the EBK condition we refer the reader to [8, 9, 12, 13].

3. Moving half-densities by the Bohmian flow

From now on we assume that H is a Hamiltonian function of the more general type

$$H = \frac{p^2}{2} + U(q, t) \quad (3.1)$$

the potential U being a C^∞ function of position q and time t . We assume that the solution ψ of the associated Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H(q, -i\hbar \nabla_q) \Psi \quad \psi(t=0) = \psi_0 \quad (3.2)$$

exists and is *uniquely* defined for all t in some interval $[-T, T]$ (or $[0, T]$). If we write ψ in polar form as

$$\psi(q, t) = \exp\left(\frac{i}{\hbar} S(q, t)\right) \sqrt{\rho(q, t)} \quad (3.3)$$

then the functions S and ρ satisfy Bohm's equations (see [3, 13])

$$\frac{\partial \rho}{\partial t} + \nabla_q(\rho \nabla_q S) = 0 \quad (3.4a)$$

$$\frac{\partial S}{\partial t} + H(q, \nabla_q S) = \frac{\hbar^2 \nabla_q^2(\sqrt{\rho})}{2\sqrt{\rho}} \quad (3.4b)$$

at all points where ρ does not vanish (we assume throughout that S and ρ are sufficiently smooth (for instance, C^∞) so that the equations (3.4) make sense). Introducing the *quantum potential*

$$U^\psi = -\frac{\hbar^2 \nabla_q^2(\sqrt{\rho})}{2\sqrt{\rho}} \quad (3.5)$$

which only depends on the initial function ψ_0 which totally determines ψ (and hence ρ and S), we can rewrite equation (3.4a) in the very suggestive form

$$\frac{\partial S}{\partial t} + H^\psi(q, \nabla_q S) = 0 \quad (3.4c)$$

where H^ψ (*'the Bohmian'*) is the sum $H + U^\psi$. Equation (3.4c) is obviously nothing more than the Hamilton–Jacobi equation for the Bohmian function H^ψ .

Remark. It is common practice among physicists to calculate ‘approximations’ to the solutions of (3.2) by ‘neglecting’ the quantum potential U^ψ and replacing the correct equation (3.4c) by its classical counterpart (2.8). However, this is indeed a risky procedure: it is not because there is a factor of order $O(\hbar^2)$ in front of the expression on the right-hand side of formula (3.5) that the quantum potential U^ψ is necessarily small. In fact, since ρ depends on \hbar it can very well happen that U^ψ ‘blows up’ at the limit $\hbar \rightarrow 0$ (see [13] for examples where this occurs). In fact, the validity of the approximation ‘ $U^\psi = 0$ ’ is closely related to that of the method of the stationary phase, when one tries to estimate the solution ψ written in integral form (as in formula (2.13) for instance). *When* the method does apply (this is the case for (2.13) when the initial wavefunction has compact support), then the main contribution at the limit $\hbar \rightarrow 0$ comes from the critical points of the generating function, and one shows that the result amounts to moving the wavefunction along the *classical trajectory* associated with the original Hamiltonian H .

Setting $t = 0$ in (3.3) the initial wavefunction can be written as

$$\psi_0(q) = \exp\left(\frac{i}{\hbar} S_0(q)\right) \sqrt{\rho_0(q)} \quad (3.6)$$

where $\rho_0 = \rho(q, 0)$ and $S_0 = S(q, 0)$ are real C^∞ functions defined on some open domain D of \mathbb{R}_q^n . Let L_0 be the graph of the gradient of S_0 ; it is the manifold

$$L_0 = \{(q, p) : p = \nabla_q S_0(q), q \in D\}. \quad (3.7)$$

L_0 is in fact a Lagrangian submanifold of the phase space $\mathbb{R}_q^n \times \mathbb{R}_p^n$, that is, it has dimension n and the canonical symplectic form

$$\Omega = dp_1 \wedge dq_1 + \cdots + dp_n \wedge dq_n$$

vanishes on any pair of tangent vectors to L_0 . We notice that since L_0 is a graph, the restriction π_0 to L_0 of the projection $\pi : (q, p) \rightarrow q$ is a diffeomorphism and (L_0, π_0) is thus a global chart.

Denote now by $(f_{t,t'}^\psi)_{t,t'}$ the time-dependent flow associated with the ‘Bohmian’ H^ψ ; $f_{t,t'}^\psi$ is thus the symplectic transformation of phase space defined by

$$(q^\psi(t), p^\psi(t)) = f_{t,t'}^\psi(q, p)$$

if and only if

$$\frac{dq^\psi}{dt} = \nabla_p H^\psi \quad \frac{dp^\psi}{dt} = -\nabla_q H^\psi \quad (3.8)$$

and $q^\psi(t') = q$, $p^\psi(t') = p$. Using the Bohmian flow thus defined we can carry the manifold L_0 in phase space to another manifold L_t . Defining

$$L_t = f_t^\psi(L_0) \quad f_t^\psi = f_{t,0}^\psi \quad (3.9)$$

we obviously have $f_{t,t'}^\psi(L_{t'}) = L_t$.

Proposition 1. The manifold L_t is a Lagrangian submanifold of $\mathbb{R}_q^n \times \mathbb{R}_p^n$ which projects diffeomorphically on $D_t = f_t^\psi(D_0)$. In fact L_t is the graph

$$L_t = \{(Q, P) : P = \nabla_Q S(Q, t)\} \quad (3.10)$$

and we have, moreover,

$$S(q^\psi(t), t) = S_0(q) + \int_0^t p \, dq - H^\psi \, dt' \quad (3.11)$$

where the integration is performed along the phase-space trajectory leading from $(q, \nabla_q S_0)$ at time $t = 0$ to $(Q, P) = (q^\psi(t), \nabla_q S(q^\psi(t), t))$ at time t .

Proof. That L_t is a Lagrangian manifold is clear, because f_t^ψ is a symplectic mapping and as such preserves the symplectic structure: $(f_t^\psi)^* \Omega = \Omega$. Formula (3.11) is a classical application of Hamilton–Jacobi theory (see [1, ch 9]): define the action function

$$\Phi(Q, t) = S_0(q) + \int_0^t p \, dq - H^\psi \, dt'$$

where the integration is performed along the trajectory from $(q, p, 0)$ to (Q, P, t) . Then

$$d\Phi(Q, t) = P \, dQ - H^\psi \, dt$$

so that we have

$$P = \frac{\partial \Phi}{\partial Q}(Q, t) \quad \frac{\partial \Phi}{\partial t} = -H^\psi(Q, P, t).$$

In particular, Φ satisfies the Hamilton–Jacobi equation (3.4c) with initial condition S_0 , and hence $\Phi = S$; formulae (3.10) and (3.11) follow. \square

Remark. The fact that L_t is itself a graph is noticeable, because, in general, Hamiltonian flows deform graphs in such a way that they become new manifolds which usually ‘bends’ after some time t , and thus are no longer graphs. This well known phenomenon is at the origin of the appearance of ‘caustics’, that is, of points of the deformed manifold who admit no neighbourhood projecting diffeomorphically on configuration space (see [1, 9, 14, 15] and the references therein). The appearance of these caustics is actually an artifact of Hamilton–Jacobi theory, related to the impossibility of finding global solutions to the Hamilton–Jacobi equation. This does not happen in our case, because we already have at hand a globally defined solution, namely the phase $S(q, t)$ of the wavefunction.

We now return to the half-density interpretation of wavefunctions. Our main result is the following.

Proposition 2. The notation being as in proposition 1, we have

$$(q^\psi(t), t) = \exp \left[\frac{i}{\hbar} \int_0^t p \, dq - H^\psi \, dt' \right] \left| \det \frac{\partial q^\psi(t)}{\partial q} \right|^{1/2} \Psi_0(q) \quad (3.12)$$

where $\partial q^\psi / \partial q$ is the Jacobian matrix; denoting by $d^n q$ the Lebesgue measure on \mathbb{R}_q^n and by $|d^n q|^{1/2}$ the associated half-density, formula (3.12) is equivalent to

$$\Psi(Q, t) |d^n Q|^{1/2} = \exp \left[\frac{i}{\hbar} \int_0^t p \, dq - H^\psi \, dt' \right] \Psi_0(q) |d^n q|^{1/2}. \quad (3.13)$$

Proof. The equivalence of (3.12) and (3.13) is clear in view of the definition of the half-density $|d^n q|^{1/2}$ (see, for instance, [19]). On the other hand, the arguments of both sides of (3.12) (or (3.13)) are equal in view of (3.11), so that all we have to prove is the equality of the moduli of both sides of (3.12). This amounts to proving that

$$\rho_0(q) = \rho(q^\psi(t), t) \left| \det \frac{\partial q^\psi(t)}{\partial q} \right| \quad (3.14)$$

which is, in fact, an immediate consequence of (3.4a): it is a classical results from fluid mechanics that if a function ρ is the solution to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla_q(\rho V) = 0$$

where $V = V(q, t)$ is some fluid velocity field, then $\rho(q, t)$ satisfies the relation

$$\rho(q, 0) = \rho(q(t), t) \left| \det \frac{\partial q(t)}{\partial q} \right|.$$

Applying this formula to (3.4a) with $V(q, t) = \partial S(q, t) / \partial q$ yields (3.13). \square

4. Semiclassical approximation

Suppose now that the quantum potential U^ψ can be neglected. Formula (3.13) then becomes in view of (3.11), as long as t is small,

$$(q(t), t) = \exp \left[\frac{i}{\hbar} \Phi(q(t), t) \right] \left| \det \frac{\partial q(t)}{\partial q} \right|^{1/2} \Psi_0(q) \quad (4.1)$$

where $\Phi = \Phi(q, t)$ is the solution of the classical Hamilton–Jacobi equation

$$\frac{\partial \Phi}{\partial t} + H(q, \nabla_q \Phi, t) = 0 \quad \Phi(q, 0) = S_0(q) \quad (4.2)$$

and $q(t)$ and $p(t)$ are the solutions of Hamilton’s equations

$$\frac{dq(t)}{dt} = \nabla_p H(q(t), p(t), t) \quad \frac{dp(t)}{dt} = -\nabla_q H(q(t), p(t), t). \quad (4.3)$$

For larger values of t , the solution to (4.2) will, in general, no longer exist. *However*, the action integral

$$W = \int_0^t p \, dq - H \, dt' \quad (4.4)$$

does, *but* it will in general be multiple valued: as discussed previously, $L(t) = f_t(L_0)$ (the image of L_0 by the flow $(f_t)_t$ determined by (4.3)) is usually no longer a graph, so that there will be several points $(q(t), P_j)$ of L_t with the same projection $q(t)$ on the configuration space \mathbb{R}_q^n . Defining the points $(q_j, p_j) \in L_0$ by $f_t(q_j, p_j) = (q(t), P_j)$ the correct formula that replaces (4.1) for arbitrary t takes into account the contributions from all the classical trajectories starting from the points (q_j, p_j) and ending at the points $(q(t), P_j) = (q(t), p_j(t))$. One then recovers Maslov’s formula for the semiclassical approximation (see [1, 9, 11, 16])

$$\Psi(q, t) = \sum_j e^{(i/\hbar)\Phi_j(x,t)} i^{\mu_j} \left| \det \frac{\partial q_j(t)}{\partial q} \right|^{-1/2} \sqrt{\rho(q, j)} \quad (4.5)$$

as long as (q, t) is not a ‘focal point’ (i.e. q is not the projection of a point of the caustic). The functions $\Phi_j(x, t)$ are given by

$$\Phi_j(q, t) = S_0(q_j) + \int_0^t L(q, q, t') \, dt' \quad (4.6)$$

where $L = pq - H$ is the Lagrangian function and the μ_j appearing as exponents in (4.5) are integers called ‘Morse indices’ of the trajectories from q_j to $q(t)$ (see [1, appendix 11]). We refer the reader to [9–11] for a thorough study of formulae (4.5) and (4.6), and of the relation between the Morse indices and the Maslov index).

5. Conclusion

The semiclassical formula (4.5) is usually obtained by quite different approaches, which, however, have in common the fact that they all make use of the method of the stationary phase. The way we have derived formula (4.5), which only makes use of proposition 2, shows that the half-density approach might be a promising one, both in standard quantum mechanics and in quantum theory of motion. We think that this method, therefore, certainly deserves further study because it might be the key to a better understanding of quantum mechanics.

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