Quantum–classical correspondence via a deformed kinetic operator

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Abstract

We propose an approach to quantum–classical correspondence based on a deformation of the momentum and kinetic operators of quantum mechanics. Making use of the factorization method, we construct classical versions of the momentum and kinetic operators which, in addition to the standard quantum expressions, contain terms that are functionals of the N-particle density. We show that this implementation of quantum–classical correspondence is related to Witten's deformation of the exterior derivative and Laplacian, introduced in the context of supersymmetric quantum mechanics. The corresponding deformed action is also shown to be related to the Fisher information. Finally, we briefly consider the possible relevance of our approach to the construction of kinetic-energy density functionals.

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1. Introduction

Since the origins of quantum mechanics there has been interest in the correspondence between quantum and classical mechanics which has continued to the present [1]. In his 1926 paper [2], Schrödinger begins with the classical Hamilton–Jacobi equation and then writes down a wavefunction equation (now known as the Schrödinger equation) without making an explicit connection between the two. A general connection was made by Van Vleck in his 1928 paper [3] and extended by Schiller [4] who modified the classical Hamilton–Jacobi equation to obtain a quantum-like formulation of classical mechanics. On the other hand, in his 1928 paper [5] Madelung begins with the wavefunction in polar form and then writes down hydrodynamic equations to obtain a classical-like formulation of quantum mechanics. This approach was extended by Bohm [6] who explicitly introduced the quantum potential, Q. One can think

of quantum–classical correspondence as 'switching off' the quantum potential term in the modified (quantum) Hamilton–Jacobi equation [7] and this approach was explicitly explored in [8]. The $Q \to 0$ and (more usual) $\hbar \to 0$ approaches to quantum–classical correspondence are discussed in [7] (see also [9]).

In this paper, we approach quantum–classical correspondence at the level of the equations of motion of an N-particle system. Recall that, by expressing the wavefunction in polar form, the Schrödinger equation can be transformed into two equations [5, 10]: a modified Hamilton–Jacobi equation in which the quantum potential, Q, appears in addition to the external potential, and a continuity equation. In this context, one formally obtains the quantum equations of motion by 'switching on' the quantum potential term in the classical Hamilton–Jacobi equation. As we review in section 2, one may similarly think of formally obtaining the classical equations of motion by 'switching on' the quantum potential term in the Schrödinger equation [7]. Either way, Q is tacitly regarded as an additional *potential* term in these approaches.

In this work we follow an alternate approach, in which Q is incorporated in the *kinetic* term. This different perspective results in a deformed kinetic operator which naturally motivates the search for a deformed momentum operator. In section 3, making use of the factorization method [11], we construct classical versions of the momentum and kinetic operators and show that, in addition to the standard quantum expressions, these operators contain terms which are functionals of the N-particle density. We show that our classical version of the momentum operator is equivalent to a certain classical momentum component, introduced by Hall in [12], which gives the best classical estimate that is compatible with simultaneous knowledge of the position of the system. In section 4, we show that our approach is formally related to Witten's deformation of the exterior derivative and Laplacian [13] (see also [14] and appendix A of [15]). In section 5, we show that the deformed momentum operator reproduces, at the action level, the quantization procedure developed by Reginatto [16], where the Schrödinger equation is derived from an information-theoretical approach based on the principle of minimum Fisher information [17]. Our conclusions are presented in section 6, where we also discuss how our work is related to that of Hall and Reginatto [18], who approach quantum–classical correspondence by introducing certain momentum fluctuations obeying an exact Heisenberg-type equality. Finally, the possible relevance of our approach to the construction of kinetic-energy density functionals (see [19, 20] and references therein) is briefly considered in the appendix.

2. Quantum–classical correspondence and the quantum potential

In the hydrodynamic formulation of quantum mechanics the quantum potential appears as an additional potential term in a modified Hamilton–Jacobi equation, which defines a classical-like description of quantum mechanics. In a complementary way, the quantum potential also appears as an additional term in a modified Schrödinger equation which defines a quantum-like description of classical mechanics [7, 8]. In this section, we briefly review these procedures.

2.1. Classical-like description of quantum mechanics

Consider a *quantum N-particle* system described by a wavefunction $\psi = \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)$ satisfying the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 \psi + V\psi, \tag{1}$$

where m_k is the mass of the kth particle and V includes interparticle and external potentials. Writing $\psi = \sqrt{\rho}\, e^{\frac{i}{\hbar}S}$, and expressing the Schrödinger equation in terms of ρ and S yields [5, 7]

$$\frac{\partial S}{\partial t} + \sum_{k=1}^{N} \frac{(\nabla_k S)^2}{2m_k} + V + Q = 0, \tag{2a}$$

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^{N} \nabla_k \cdot \left(\rho \frac{\nabla_k S}{m_k} \right) = 0, \tag{2b}$$

where Q is the *quantum potential*

$$Q = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \frac{\nabla_k^2 \sqrt{\rho}}{\sqrt{\rho}}.$$

The system of coupled equations (2) comprises a modified Hamilton–Jacobi equation—in which Q appears in addition to the classical potential V—and a continuity equation. In this way, it is the quantum potential that introduces, in the context of equation (2a), all non-classical effects of quantum mechanics, such as superposition, interference and entanglement [8, 10].

2.2. Quantum-like description of classical mechanics

In this case, one starts from a *classical N-particle system* whose action function S is governed by the usual Hamilton–Jacobi equation $\frac{\partial S}{\partial t} + \sum_{k=1}^{N} \frac{(\nabla_k S)^2}{2m_k} + V = 0$ [21]. The associated (local) momentum is given by $\mathbf{p}_k = m_k \frac{d\mathbf{r}_k}{dt} = \nabla_k S$. Consider a distribution function ρ defining an ensemble of such trajectories, and satisfying the continuity equation $\frac{\partial \rho}{\partial t} + \sum_{k=1}^{N} \nabla_k \cdot \left(\rho \frac{\nabla_k S}{m_k} \right) = 0$. One can then introduce the so-called 'classical wavefunction' [7, 8]

$$\psi_{cl} = \sqrt{\rho}\, e^{iS/\hbar}, \tag{3}$$

which can be shown to satisfy the modified Schrödinger equation

$$i\hbar \frac{\partial \psi_{cl}}{\partial t} = \left(-\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 + V \right) \psi_{cl} - Q\psi_{cl}. \tag{4}$$

Note that, because of the last term, equation (4) is *nonlinear*. In this way, the quantum potential term in equation (4) completely eliminates the quantum characteristics of the usual (linear) Schrödinger equation, giving rise to a purely classical behaviour, as described by the Hamilton–Jacobi equation.

3. Classical versions of momentum and kinetic operators

The interpretation of Q as an additional *potential* term in the particle's equation of motion has far-reaching consequences, as the hydrodynamical formulation of quantum mechanics shows. Notwithstanding, both equations (2a) and (4) allow an alternative interpretation of Q as a deformation of the *kinetic* term in the corresponding equation of motion. In particular, one can readily interpret the additional term in equation (4) as a deformation of the kinetic operator in quantum mechanics,

$$-\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 \rightarrow -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 - Q.$$

This motivates the definition of a classical version of the kinetic operator as

$$K_{\text{cl}} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 - Q. \tag{5}$$

This change of perspective motivates the search for a classical version of the momentum operator to be associated with K_{cl}. We now develop this idea.

In the spirit of the factorization method in quantum mechanics [11], we assume a factorization of equation (4) as

$$\left(-\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 - Q\right)\psi = \sum_{k=1}^{N} \frac{1}{2m_k}(-i\hbar\nabla_k - \mathbf{g}_k)\cdot(-i\hbar\nabla_k + \mathbf{g}_k)\psi, \tag{6}$$

where $\mathbf{g}_k$ is a function to be determined. Expanding this expression yields

$$\sum_{k=1}^{N} \frac{1}{m_k}\left(i\hbar\nabla_k\cdot\mathbf{g}_k + \mathbf{g}_k^2 + \hbar^2\frac{\nabla_k^2\sqrt{\rho}}{\sqrt{\rho}}\right)\psi = 0.$$

This suggests that we choose a purely imaginary $\mathbf{g}_k$, of the form $\mathbf{g}_k = i\boldsymbol{\alpha}_k$ (with $\boldsymbol{\alpha}_k$ real) which yields

$$\sum_{k=1}^{N} \frac{1}{m_k}\left(\hbar\nabla_k\cdot\boldsymbol{\alpha}_k + \boldsymbol{\alpha}_k^2 - \hbar^2\frac{\nabla_k^2\sqrt{\rho}}{\sqrt{\rho}}\right)\psi = 0.$$

Now we note that

$$\frac{1}{\sqrt{\rho}}\nabla_k^2\sqrt{\rho} = \nabla_k\cdot\left(\frac{1}{\sqrt{\rho}}\nabla_k\sqrt{\rho}\right) - \nabla_k\left(\frac{1}{\sqrt{\rho}}\right)\cdot\nabla_k(\sqrt{\rho})$$

$$= \nabla_k\cdot\left(\frac{1}{\sqrt{\rho}}\nabla_k\sqrt{\rho}\right) + \left(\frac{1}{\sqrt{\rho}}\nabla_k\sqrt{\rho}\right)^2.$$

Substituting in the above equation yields the following condition on $\boldsymbol{\alpha}_k$:

$$\sum_{k=1}^{N} \frac{1}{m_k}\left[\hbar\nabla_k\cdot\boldsymbol{\alpha}_k + \boldsymbol{\alpha}_k^2 - \hbar\nabla_k\cdot\left(\frac{\hbar}{\sqrt{\rho}}\nabla_k\sqrt{\rho}\right) - \left(\frac{\hbar}{\sqrt{\rho}}\nabla_k\sqrt{\rho}\right)^2\right]\psi = 0.$$

This is immediately fulfilled by the choice

$$\boldsymbol{\alpha}_k = \hbar\frac{\nabla_k\sqrt{\rho}}{\sqrt{\rho}} = \frac{\hbar}{2}\frac{\nabla_k\rho}{\rho},$$

with $k = 1, \ldots, N$.

Bearing in mind equation (6), the discussion above motivates the definition of a classical version of the momentum operator as

$$\mathbf{P}_{\text{cl}} = \mathbf{P} + i\frac{\hbar}{2}\frac{\nabla\rho}{\rho}, \tag{7}$$

and correspondingly, $\mathbf{P}_{\text{cl}}^{\dagger} = \mathbf{P} - i\frac{\hbar}{2}\frac{\nabla\rho}{\rho}$. Here, $\mathbf{P} = -i\hbar\nabla$ is the usual N-particle quantum mechanical momentum operator, with $\mathbf{P} = (\mathbf{P}_1, \ldots, \mathbf{P}_N)$ and $\nabla = (\nabla_1, \ldots, \nabla_N)$.

It is crucial to note that the N-particle density ρ in the expressions of $\mathbf{P}_{\text{cl}}$ and $\mathbf{P}_{\text{cl}}^{\dagger}$ is that associated with the wavefunction ψ of the system (so that $\rho = \psi^*\psi$), regardless of the function on which $\mathbf{P}_{\text{cl}}$ and $\mathbf{P}_{\text{cl}}^{\dagger}$ operate; the notation $\mathbf{P}_{\text{cl}}^{\dagger}$ is to be understood in this context (see also below). Thus, the operator $\mathbf{P}_{\text{cl}}$ is a functional of the N-particle density and, in particular, we can write (for the wavefunction of the system)

$$\mathbf{P}_{\text{cl}}\psi = -i\hbar\left(\nabla - \frac{1}{2}\frac{\nabla(\psi^*\psi)}{\psi^*\psi}\right)\psi,$$

so that the action of $\mathbf{P}_{cl}$ is nonlinear in ψ. In this way, the notation $\mathbf{P}_{cl}^{\dagger}$ is not to be interpreted as the Hermitian conjugate of a (standard) linear operator in ψ. Nonetheless, $\mathbf{P}_{cl}$ and $\mathbf{P}_{cl}^{\dagger}$ are complementary in that $\mathbf{P}_{cl}$ arises naturally from the exterior derivative while $\mathbf{P}_{cl}^{\dagger}$ arises naturally from its coderivative (see section 4). Also, the last term in equation (7) can be interpreted as representing momentum fluctuations (see section 6) so that, in a certain sense, $\mathbf{P}_{cl}$ and $\mathbf{P}_{cl}^{\dagger}$ are statistically conjugate.

The classical version of the kinetic operator of equation (5) can then be expressed as

$$K_{cl} = \sum_{k=1}^{N} \frac{1}{2m_k} \left(\mathbf{P}_{cl}^{\dagger} \right)_k \cdot (\mathbf{P}_{cl})_k. \tag{8}$$

In the limiting case of a one-particle system ($N = 1$), this simplifies to

$$K_{cl} = \frac{1}{2m} \mathbf{P}_{cl}^{\dagger} \cdot \mathbf{P}_{cl}.$$

Note that $\mathbf{P}_{cl}$ plays the role of a classical version of the momentum operator, in the sense that it is associated with the kinetic term K_{cl} appearing in the modified Schrödinger equation (4). As equation (4) is nonlinear, we see that, as a matter of fact, it is mandatory for $\mathbf{P}_{cl}$ to be nonlinear in ψ.

It is interesting to note that the action of $\mathbf{P}_{cl}$ on the wavefunction ψ of the system is given by

$$\mathbf{P}_{cl}\psi = \hbar \, \mathrm{Im} \left(\frac{\nabla \psi}{\psi} \right) \psi, \tag{9}$$

as a straightforward calculation shows. Therefore, writing $\psi = \sqrt{\rho} \, e^{iS/\hbar}$, we find

$$\mathbf{P}_{cl}\psi = \nabla S \, \psi. \tag{10}$$

As discussed in section 2.2, given the 'classical wavefunction' $\psi_{cl} = \sqrt{\rho} \, e^{iS/\hbar}$, the quantity ∇S can be interpreted as the local momentum associated with an ensemble of trajectories. This reinforces our interpretation of $\mathbf{P}_{cl}$ as a classical version of the momentum operator. Further justification on this point can be given by noting that

$$\langle \mathbf{P} \rangle_{\psi} = \langle \mathbf{P}_{cl} \rangle_{\psi}, \tag{11}$$

where $\langle A \rangle_{\psi} = \int \psi^* A \psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_N$ is the expectation value of the operator A (here in position representation) in the state ψ.

From a different perspective, an equivalent definition of a classical momentum, $\mathcal{P}_{cl}$, associated with a given wavefunction ψ, was introduced in [12]. In these works, Hall defines a state-dependent decomposition of the momentum observable P into 'classical' and 'nonclassical' components $P = \mathcal{P}_{cl} + \mathcal{P}_{nc}$. The classical component $\mathcal{P}_{cl}(\mathbf{r})$ corresponds to the best possible estimate of the momentum which is compatible with simultaneous knowledge of the position of the system, and is given by [12]

$$\mathcal{P}_{cl}(\mathbf{r}) = \hbar \, \mathrm{Im} \left(\frac{\nabla \psi(\mathbf{r})}{\psi(\mathbf{r})} \right). \tag{12}$$

In this way, the classical version of the momentum operator $\mathbf{P}_{cl}$ of equation (7) is essentially equivalent to the classical momentum function $\mathcal{P}_{cl}(\mathbf{r})$ of equation (12). We also note that equation (11) was already obtained in [12] with $\mathcal{P}_{cl}$ in the place of $\mathbf{P}_{cl}$.

Let us now compare the action of $\mathbf{P}$ and $\mathbf{P}_{cl}$ on some particular one-dimensional examples. For a plane wave $\psi = e^{\frac{i}{\hbar} p_0 x}$ (p_0 constant), we see that the actions of $\mathbf{P}_{cl}$ and $\mathbf{P}$ coincide, so that $\mathbf{P}_{cl}\psi = \mathbf{P}\psi = p_0 \psi$. On the other hand, it follows from equation (7) that any ψ with a nontrivial probability distribution $\rho = \psi^* \psi$ will lead to different results under the action of $\mathbf{P}$ and $\mathbf{P}_{cl}$.

Consider, for example, a Gaussian wave packet with width σ, $\psi(x) = \mathrm{e}^{-(x-x_0)^2/(2\sigma)^2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_0 x}$, which corresponds to a state with uncertainties in position and momentum minimizing the Heisenberg uncertainty principle. Note that, although ψ is as close we can get to a quantum state with definite position x_0 and momentum p_0, it is not an eigenstate of $\mathbf{P} = -\mathrm{i}\hbar\partial_x$ and therefore does not correspond to a state of definite momentum. On the other hand, we readily see that $\mathbf{P}_{\mathrm{cl}}\psi = p_0\psi$. This is a consequence of the fact that $\mathbf{P}_{\mathrm{cl}}$ is only concerned with the local momentum (in the sense above) associated with ψ.

4. Witten's approach to supersymmetric quantum mechanics

Some time ago, Witten constructed a connection between supersymmetric quantum mechanics and Morse theory [13] which has been very influential. Central to Witten's approach [13] is the deformation of the exterior derivative, d,

$$d \to d_\lambda = \mathrm{e}^{-\lambda f} d\, \mathrm{e}^{\lambda f}, \qquad \lambda \in \mathbb{R} \tag{13}$$

and correspondingly, the deformation of its coderivative, $\delta = d^\dagger$, $\delta \to \delta_\lambda = \mathrm{e}^{\lambda f}\delta\,\mathrm{e}^{-\lambda f}$ (see also [14] and appendix A of [15]). We note that, by choosing $f = -\frac{1}{2}\ln\rho$, the action of d_λ on scalar functions (i.e., 0-forms) is given by

$$-\mathrm{i}\hbar\nabla^{(\lambda)} = -\mathrm{i}\hbar\nabla + \mathrm{i}\hbar\frac{\lambda}{2}\frac{\nabla\rho}{\rho}, \tag{14}$$

where, as before, ∇ denotes the $3N$-dimensional gradient and we employ a vector notation for the outcome of d and d_λ when applied to a scalar function[4].

This suggests (cf equation (7)) that we define a deformed momentum operator, $\mathbf{P}_\lambda$, by

$$\mathbf{P}_\lambda = \mathbf{P} + \mathrm{i}\lambda\frac{\hbar}{2}\frac{\nabla\rho}{\rho}, \tag{15}$$

and correspondingly, $\mathbf{P}_\lambda^\dagger = \mathbf{P} - \mathrm{i}\lambda\frac{\hbar}{2}\frac{\nabla\rho}{\rho}$. Given the relationship between the factorization method and supersymmetric quantum mechanics [11], this connection between $\mathbf{P}_\lambda$ and d_λ is, in fact, not unexpected. Once again, it is crucial to bear in mind that the density ρ in equation (15) is that for the wavefunction ψ of the system, regardless of the function on which $\mathbf{P}_\lambda$ (and $\mathbf{P}_\lambda^\dagger$) operate and the notation $\mathbf{P}_\lambda^\dagger$ is to be understood in this context. Also, the same observations made for $\mathbf{P}_{\mathrm{cl}}$ concerning its nonlinearity in ψ also apply to $\mathbf{P}_\lambda$. For $\lambda = 0$, $\mathbf{P}_\lambda$ recovers the usual quantum momentum while for $\lambda = 1$, $\mathbf{P}_\lambda$ recovers the classical version, $\mathbf{P}_{\mathrm{cl}}$, of the previous section. As λ increases from 0 to 1, one can envisage a scenario in which quantum mechanics gradually assumes classical effects.

Also central to Witten's approach [13] is the deformation of the Laplacian, L,

$$L \to L_\lambda = (d_\lambda + \delta_\lambda)^2. \tag{16}$$

L_λ is the natural Laplacian corresponding to d_λ and δ_λ. When restricted to scalar functions, it is not difficult to show that L_λ satisfies $\frac{\hbar^2}{2m}L_\lambda\big|_{\substack{\text{scalar}\\\text{functions}}} = \frac{1}{2m}\mathbf{P}_\lambda^\dagger \cdot \mathbf{P}_\lambda$. This suggests (cf equation (8)) that we define a deformed kinetic operator, K_λ, by

$$K_\lambda = \sum_{k=1}^{N}\frac{1}{2m_k}\left(\mathbf{P}_\lambda^\dagger\right)_k \cdot (\mathbf{P}_\lambda)_k. \tag{17}$$

In the limiting case of a one-particle system ($N = 1$), this simplifies to

$$K_\lambda = \frac{1}{2m}\mathbf{P}_\lambda^\dagger \cdot \mathbf{P}_\lambda.$$

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[4] This amounts to identifying 1-forms with vector fields via the isomorphism induced by the Euclidean metric in $\mathbb{R}^{3N}$, so that the actions of d and d_λ on a scalar function φ are mapped into $\nabla\varphi$ and $\nabla^{(\lambda)}\varphi$, respectively.

For $\lambda = 0$, K_λ recovers the usual quantum kinetic operator, while for $\lambda = 1$, K_λ recovers its classical version, K_{cl}, of the previous section.

We note that a related connection between the quantum potential and supersymmetry was considered in [14], where the quantum potential is obtained from a Riemann–Cartan–Weyl geometry and deformed Laplacians are associated with generators of a family of diffusion processes.

5. Deformed action and Fisher information

The Fisher information, I_F, was introduced in statistical analysis as a measure of the intrinsic accuracy of an estimate [17]. Given an N-particle system with associated probability density ρ, it has been shown [16] that I_F is directly proportional to the average of Q. For simplicity, we restrict ourselves to the case $N = 1$, where I_F is given by

$$I_F = \int \frac{1}{\rho} \, (\nabla \rho)^2 \, \mathrm{d}\mathbf{r} \, \mathrm{d}t.$$

We note that, in this case, the Fisher information and the Weizsäcker term, W, in Density Functional Theory [22] are directly proportional with $W = \frac{\hbar^2}{8m} I_F$.

In order to relate the deformed momentum operator $\mathbf{P}_\lambda$ to Fisher information, we recall that, from a field theoretical viewpoint, the Schrödinger equation can be derived from the action [7]

$$\mathcal{S} = \int \left[\mathrm{i}\frac{\hbar}{2} \left(\psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi \right) - \frac{1}{2m} (\mathbf{P}\psi)^* \cdot (\mathbf{P}\psi) - V \psi^* \psi \right] \mathrm{d}\mathbf{r} \, \mathrm{d}t, \quad (18)$$

where $\mathbf{P} = -\mathrm{i}\hbar\nabla$ (as above).

When we substitute $\mathbf{P} \to \mathbf{P}_{cl}$ in equation (18), we obtain the classical action

$$\mathcal{S}_{cl} = \int \left[\mathrm{i}\frac{\hbar}{2} \left(\psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi \right) - \frac{1}{2m} (\mathbf{P}_{cl}\psi)^* \cdot (\mathbf{P}_{cl}\psi) - V \psi^* \psi \right] \mathrm{d}\mathbf{r} \, \mathrm{d}t, \quad (19)$$

and for $\psi = \sqrt{\rho} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S}$, this expression becomes

$$\mathcal{S}_{cl} = -\int \rho \left(\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V \right) \mathrm{d}\mathbf{r} \, \mathrm{d}t, \quad (20)$$

which gives rise (upon variation of ρ and S) to the *classical* Hamilton–Jacobi equation $\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V = 0$, along with the continuity equation $\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = 0$.

It is then natural to consider the deformed action

$$\mathcal{S}_\lambda = \int \left[\mathrm{i}\frac{\hbar}{2} \left(\psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi \right) - \frac{1}{2m} (\mathbf{P}_\lambda\psi)^* \cdot (\mathbf{P}_\lambda\psi) - V \psi^* \psi \right] \mathrm{d}\mathbf{r} \, \mathrm{d}t, \quad (21)$$

associated with the deformed momentum $\mathbf{P}_\lambda$ introduced above. For $\psi = \sqrt{\rho} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S}$, a straightforward calculation yields

$$\mathcal{S}_\lambda = -\int \left[\rho \left(\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V \right) + \xi \frac{1}{\rho} (\nabla \rho)^2 \right] \mathrm{d}\mathbf{r} \, \mathrm{d}t, \quad (22)$$

with

$$\xi = \frac{\hbar^2 (1 - \lambda)^2}{8m}.$$

It is interesting to note that this equation is the starting point of [16] to show that the Schrödinger equation may be derived from an information-theoretical approach based on the principle of minimum Fisher information[5]. This can be seen as follows. In equation (22), the Lagrange

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[5] Note that the parameter ξ in equation (22) is a function of λ and is thus far free. To avoid confusion, we note that in [16] the author uses a slightly different notation, with our ξ corresponding to his $\frac{\lambda}{m}$.

multiplier ξ imposes a constraint to the purely classical Hamilton–Jacobi action (20) which enforces the minimization of I_F for a given S [23]. As a result, $\mathcal{S}_\lambda$ yields—upon variation of ρ and S—the continuity equation $\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = 0$ (for any value of ξ), along with the modified Hamilton–Jacobi equation $\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V + \xi \left(-4 \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) = 0$ which, as we have seen, is equivalent to the Schrödinger equation for $\xi = \frac{\hbar^2}{8m}$ (in our case, this corresponds to $\lambda = 0$).

6. Discussion and conclusions

We have proposed an approach to quantum–classical correspondence via deformed momentum and kinetic operators. We started by reviewing the role played by the quantum potential, Q, in providing quantum–classical correspondence at the level of the equations of motion of an N-particle system. However, instead of regarding Q as an additional *potential* term, we have regarded Q as resulting from a deformation of the *kinetic* term in the corresponding equation of motion. We introduced a deformed momentum operator, $\mathbf{P}_\lambda$, which is related to Witten's deformation of the exterior derivative, and a deformed kinetic operator, K_λ, which is related to Witten's deformation of the Laplacian. The deformed momentum and kinetic operators each contain the standard quantum mechanical expression and an additional term which is a functional of the N-particle density.

We have shown that our approach leads to connections to the factorization method, to Witten's approach to supersymmetric quantum mechanics and to the Fisher information, and each of these might lead to more general formalisms.

We note that from a different perspective, Hall and Reginatto [18] approach quantum–classical correspondence by introducing momentum fluctuations which scale inversely with the uncertainty in position, so that the assumption of an exact uncertainty principle leads from the classical equations of motion to the Schrödinger equation. In this context, it may be seen that the momentum fluctuations introduced in [18] are captured, in our formalism, by the last term of equation (7). It is interesting to note that, although Hall and Reginatto approach quantum–classical correspondence from a different perspective, there are significant similarities to our approach in that we also obtain a modified kinetic term and a classical version of the quantum mechanical momentum, as discussed in section 3.

Acknowledgments

Appendix. A brief note on kinetic-energy density functionals

As noted in section 5, our approach is related to the Fisher information and this concept has given rise to several applications in Density Functional Theory [24, 25]. Density Functional Theory is, in principle, an exact physical theory (within the framework of the Born–Oppenheimer approximation); the total energy and other properties are expressed as functionals of the one-electron density which is the basic variable. We conclude by suggesting a way in which our approach might be relevant to the construction of kinetic-energy density functionals (see [19, 20] and references therein).

We write the N-electron wavefunction as $\psi = \sqrt{\rho}\, e^{\frac{i}{\hbar} S}$, where $\rho = \rho(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the N-electron density. Recall that $\mathbf{P}_{cl}$ in equation (7) contains the standard quantum mechanical expression and an additional term which is a functional of the N-electron density. For

N particles of mass m (which we can take as the electron mass) our construction of the classical version of the kinetic operator in equation (8) yields $K_{cl} = \frac{1}{2m}\mathbf{P}_{cl}^{\dagger} \cdot \mathbf{P}_{cl}$, where the scalar product implicitly contains a sum over N particles. On the other hand, a simple (and physically reasonable) construction of a kinetic operator, also built from $\mathbf{P}_{cl}$ and $\mathbf{P}_{cl}^{\dagger}$, is $K' = \frac{1}{2m}\frac{\mathbf{P}_{cl}^{2} + \mathbf{P}_{cl}^{\dagger 2}}{2}$ (which also implicitly contains sums over N particles). A straightforward calculation yields

$$K' = K - \frac{\hbar^2}{8m}\frac{[\boldsymbol{\nabla}\rho(\mathbf{r}_1, \ldots, \mathbf{r}_N)]^2}{[\rho(\mathbf{r}_1, \ldots, \mathbf{r}_N)]^2}. \tag{A.1}$$

This then yields

$$\langle K \rangle_{\psi} = \langle K' \rangle_{\psi} + \frac{\hbar^2}{8m}\int \frac{(\boldsymbol{\nabla}\rho(\mathbf{r}_1, \ldots, \mathbf{r}_N))^2}{\rho(\mathbf{r}_1, \ldots, \mathbf{r}_N)}\,\mathrm{d}\mathbf{r}_1 \cdots \mathrm{d}\mathbf{r}_N, \tag{A.2}$$

where $\langle A \rangle_{\psi}$ represents (as before) the expectation value of a given operator A in the state ψ.

The average kinetic energy is thereby expressed as the sum of two terms: the average of a kinetic-energy term constructed from the classical version of the momentum operator plus a $3N$-dimensional analogue of the Weizsäcker term. The kinetic-energy density functional is typically expressed as a linear combination of Thomas–Fermi and Weizsäcker terms [22, 20] and it would be interesting if, upon reduction to an expression in which the one-electron density is the basic variable, equation (A.2) were to yield an expression of similar form. We note that Kohout has recently considered a related reduction for the $3N$-dimensional quantum potential [26].

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