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Form of the quantum potential for use in hydrodynamic equations for semiconductor device modeling

D. K. Ferry and Jing-Rong Zhou
Center for Solid State Electronics Research, Arizona State University, Tempe, Arizona 85287-6206

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We solve a form of the Bloch equation for the density matrix in a manner that identifies a "quantum" correction to the classical potential. This correction is given by the difference between the Bohm self-potential and a form of the Wigner potential that have both been used in previous simulations of semiconductor devices. The net potential appearing in the density is then a nonlocally smoothed average of the total semiclassical potential, which itself is composed of the classical potential and the quantum correction. However, the effective potential, which appears in hydrodynamic equations for device modeling, is shown to be the difference between this nonlocally smoothed potential and the local value of the potential. The various definitions that have appeared in the literature for the quantum potential and the effective potential are compared and it is demonstrated how a connection exists among these various definitions.

INTRODUCTION

The development of quantum corrections to statistical thermodynamics, especially in equilibrium, has a rich and old history. Wigner,[1] in his introduction and discussion of the Wigner function itself, introduced a quantum-mechanical correction to the variation of the distribution function (and hence the density) in terms of higher-order derivatives of the potential itself. He showed that these higher-order derivatives contributed a correction term to the energy of the ensemble; this correction has come to be known as a form of a quantum potential. One desire for such a potential lies in the extension of the hydrodynamic equations, used extensively for semiconductor modeling,[2-4] to represent the effects of quantum mechanics without having to go to extensive solutions of exact quantum-mechanical models.[5-9] These modified hydrodynamic equations, in which some form of quantum potential has been introduced, have been used to model high electron mobility transistors (HEMT's), metal semiconductor field-effect transistors (MESFET's), tunneling structures, and simple n^+-n-n^+ structures.

Unfortunately, there is no consensus as to the form of the quantum potential to be utilized in the hydrodynamic equations. Discussion of the quantum corrections, as a potential, began with the Bohm potential[10]

$$U_B = -\frac{\hbar^2}{2m\sqrt{n}}\frac{\partial^2\sqrt{n}}{\partial x^2} , \tag{1}$$

where $\sqrt{n} = |\Psi(x,t)|$ represents the magnitude of the wave function for which Schrödinger's equation must be solved. The Bohm potential represents a *field*, through which the particle interacts with itself quantum mechanically.[10] The role of this potential on the propagation of wave packets has been studied extensively recently.[11,12]

On the other hand, Iafrate, Grubin, and Ferry[5] derived a form of the potential using moments of the Wigner function for a "pure" state. This resulted in

$$U_W = -\frac{\hbar^2}{8m}\frac{\partial^2(\ln n)}{\partial x^2} . \tag{2}$$

This form of the Wigner potential (2) is better thought of as a quantum *pressure* term, which works to modify the actual potential to allow charge penetration into the classically forbidden region of the potential. While the functional form of the quantum potential differs between (1) and (2), the absolute magnitude is actually different by only a numerical factor of order unity (in the range 1–2) in most cases. It is the latter form that has found the most use in device modeling. Equation (2) has been used in many device models,[7,8] and a form in which (2) is reduced by a factor of $\frac{1}{3}$ has been used as well,[6,13] although the Bohm potential (1) is often added to the equations so that *two* quantum potentials are present.

Both of the above potentials are strictly derived for pure states, and there is a significant difference of opinion as to the correct form for a statistical ensemble. Bohm, in his original work,[10] felt that the ensemble would expand to a form quite similar to the wave function, and therefore the form of (1) would carry through. Ancona and Iafrate[13] expanded the potential, following the development of Wigner,[1] and obtained an expansion in terms of the ratio of the thermal wavelength to the characteristic length over which the potential varied. This expansion treated the latter ratio as a small quantity, and obtained a reduction of (2) by a factor of $\frac{1}{3}$ as mentioned above. More recently, Grubin *et al.*[14] working with the density matrix, achieved the same result, again in an expansion of the mentioned small ratio. Unfortunately, simulations by the latter authors clearly show that the quantum potential is most important exactly in those regions in which the expansion ratio is not small. It is clear from this latter work that expansions in an assumed parameter, such as the ratio of the thermal wavelength to the characteristic distance over which the potential varies, cannot be used to find the quantum potential, since this parameter is clearly not small in the most important regions, and such series are unlikely to converge. This arises from the fact that such expansions result in *local point functions* in classical mechanics sense, whereas the quantum mechanics appear as nonlocal, and diffusive,

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type forces.[15]

The search to find an *effective* potential with which quantum systems can be solved in a semiclassical manner is in fact broader than the above discussion. We may think of the problem as seeking a potential $\bar{V}$ that replaces the classical potential V so that

$$e^{-\beta V} \rightarrow \exp(-\beta \bar{V}) \tag{3}$$

describes adequately the density variation in the quantum system. The above discussion of the quantum potential can be thought of as seeking an additional term that can be added to the classical potential to produce the desired effects. However, Feynman and Hibbs[16] suggested a variational approach by which the classical potential would be weighted by a Gaussian spreading function. Later work by Feynman and Kleinert[17] extended this to the development of a general variational form for the effective potential, as

$$V \rightarrow \frac{1}{\beta} \ln \left[\frac{\sinh(\beta\Omega/2)}{(\beta\Omega/2)} \right] + V_a(x_0) - \tfrac{1}{2}\Omega^2 a^2 , \tag{4}$$

where

$$V_a(x_0) = \frac{1}{\sqrt{2\pi a^2}} \int \exp\left[-\frac{1}{2a^2}(x-x_0)^2 \right] V(x)\, dx \tag{5}$$

and

$$\Omega^2(x_0) = \frac{\partial^2 V_a}{\partial x_0^2} = 2\frac{\partial V_a}{\partial a^2} \tag{6}$$

is found from an extremal principle. Other variational forms have also been suggested,[18] but these differ from (4) only in slight details. In this form, the second term on the right-hand side of (4) is a nonlocal smoothing function (in a sense representing the role of quantum diffusion in the classical potential), while the other two terms form an additive contribution in the spirit of the potentials discussed above. In fact, the leading term on the right-hand side of (4) involves the second derivative of the (smoothed) potential in a manner suggestive of the form used by Wigner.

In this paper, we develop a more general form for the quantum potential in an asymptotic limit (to be described later) and in the semiclassical limiting process for which the hydrodynamic equations are appropriate. This is achieved by actually solving a defining differential equation, and not by a series expansion of the potential and its derivatives. The quantum potential is found to be a *nonlocal* quantity, as expected from quantum mechanics. However, the result is functionally similar to (1) and (2), yet has structure quite similar to the variation potential (4). In the next section, we develop the Bloch equation for the density matrix and the limiting constraints imposed upon this equation in achieving the lowest hydrodynamic equations. The third section is then devoted to the solution for the quantum potential in the asymptotic limit. Finally, we discuss the hydrodynamic equations themselves.

THE DENSITY MATRIX AND THE BLOCH EQUATION

Whether one begins with the coordinate representation, or with a mixed coordinate-momentum representation appropriate for the Wigner distribution function,[1] the natural starting place for a discussion of a statistical ensemble remains the density matrix $\rho(\mathbf{x},\mathbf{x}',t)$. The equation of motion for this quantity is the Liouville equation, and moments of this latter equation have been developed by a variety of authors; this has recently been done in the context of the quantum potential by Grubin and co-workers.[6,14] To facilitate the present approach, we shall introduce a change of coordinates to the "center-of-mass" reference frame through

$$\mathbf{R} = \tfrac{1}{2}(\mathbf{x}+\mathbf{x}'), \quad \mathbf{s} = \mathbf{x}-\mathbf{x}' . \tag{7}$$

This leads to

$$\rho(\mathbf{x},\mathbf{x}',t) \rightarrow \rho\left[\mathbf{R}+\frac{\mathbf{s}}{2}, \mathbf{R}-\frac{\mathbf{s}}{2}, t \right] . \tag{8}$$

As mentioned, the equation of motion arises from the Liouville equation. However, this equation of motion represents the time development of the density matrix. The adjoint equation is usually used to find the equilibrium ensemble. For a statistical ensemble, we normally assume that the density varies approximately as $\exp(-\beta\varepsilon)$, with $\beta = 1/k_B T_e$, and this then leads to the Bloch equation,[13] in the center-of-mass coordinates,

$$\frac{\partial\rho}{\partial\beta} = \left\{ \frac{\hbar^2}{8m}\nabla^2 + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{s}^2} \right\}\rho - [\cosh(\tfrac{1}{2}\mathbf{s}\cdot\nabla)V(\mathbf{R})]\rho , \tag{9}$$

where

$$[\cosh(\tfrac{1}{2}\mathbf{s}\cdot\nabla)V] = \frac{1}{2}\left[V\left[\mathbf{R}+\frac{\mathbf{s}}{2}\right] + V\left[\mathbf{R}-\frac{\mathbf{s}}{2}\right] \right] . \tag{10}$$

Here, $\partial/\partial\mathbf{s}$ is a short-hand notation for the gradient with respect to the difference coordinate, and the ∇ operator refers to the center coordinate $\mathbf{R}$.

The density matrix has the usual characteristics that, in the limit $\mathbf{s}\rightarrow 0$, it becomes the normal density $n(\mathbf{R})$. To better understand the limitations we shall impose upon the development of (9), we first discuss the equation of motion for the density matrix, which is obtained from the Liouville equation as

$$i\hbar\frac{\partial\rho}{\partial t} = -\frac{\hbar^2}{m}\frac{\partial^2\rho}{\partial\mathbf{R}\partial\mathbf{s}} + 2[\sinh(\tfrac{1}{2}\mathbf{s}\cdot\nabla)V]\rho , \tag{11}$$

where the last term arises from the same source as (10), except with a negative sign appropriate to the commutator of ρ with H, rather than the positive sign arising from the anticommutator used in the Bloch equation. We note that this leads to only odd-order derivatives of the potential, which are fully reversible (the even derivatives are not time reversible).[15] If we now take the limit as $\mathbf{s}\rightarrow 0$, we obtain

$$i\hbar\frac{\partial n}{\partial t} = \lim_{\mathbf{s}\rightarrow 0}\left[-\frac{\hbar^2}{m}\frac{\partial^2\rho}{\partial\mathbf{R}\partial\mathbf{s}} \right] , \tag{12}$$

which is recognizable as the continuity equation if we require

$$\lim_{s\to 0}\left[-i\hbar\frac{\partial\rho}{\partial \mathbf{s}}\right]=\mathbf{p}_d n(\mathbf{R}) . \tag{13}$$

Similarly, we can develop the second moment equation by taking the derivative of (11) with respect to s, and then passing to the limit. This gives

$$\frac{\partial}{\partial t}[\mathbf{p}_d n(\mathbf{R})]=\frac{\hbar^2}{m}\nabla\cdot\left[\lim_{s\to 0}\frac{\partial}{\partial \mathbf{s}}\frac{\partial}{\partial \mathbf{s}}\rho\right]-n(\mathbf{R})\nabla V . \tag{14}$$

The first term on the right-hand side is the normal divergence of the "momentum-pressure" tensor in the classical limit. As is often done in the semiclassical case, we approximate this by taking the pressure tensor as an isotropic scalar quantity (the tensor is diagonal), so that (14) becomes

$$\frac{\partial}{\partial t}[\mathbf{p}_d n(\mathbf{R})]=\frac{\hbar^2}{2m}\nabla\left[\lim_{s\to 0}\frac{\partial^2}{\partial \mathbf{s}^2}\rho\right]-n(\mathbf{R})\nabla V . \tag{15}$$

This leads us to recognize that

$$-\frac{\hbar^2}{2m}\lim_{s\to 0}\frac{\partial^2}{\partial \mathbf{s}^2}\rho=\langle\varepsilon\rangle n(\mathbf{R}) . \tag{16}$$

Equations (13) and (16) constitute a pair of "boundary" conditions which will need to be imposed upon our solution to (9) for the equilibrium density matrix.

In solving (9), we first note that the potential driving term can be taken to be an integrating factor, so that we can rewrite this equation as

$$\frac{\partial}{\partial\beta}[e^{\beta W}\rho]=e^{\beta W}\left\{\frac{\hbar^2}{8m}\nabla^2+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{s}^2}\right\}\rho , \tag{17}$$

where

$$W(\mathbf{R},\mathbf{s})=[\cosh(\tfrac{1}{2}\mathbf{s}\cdot\nabla)V] . \tag{18}$$

We now assert that the last term can be written in terms of a new function

$$F(\mathbf{R},\mathbf{s})\rho=\left\{\frac{\hbar^2}{8m}\nabla^2+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{s}^2}\right\}\rho , \tag{19}$$

so that (17) can now be solved to give

$$\rho(\mathbf{R},\mathbf{s})=A\exp\left\{-\beta W(\mathbf{R},\mathbf{s})+\int^{\beta}F(\mathbf{R},\mathbf{s})d\beta'\right\} . \tag{20}$$

Our problem now is to solve for $F(\mathbf{R},\mathbf{s})$.

To proceed, it is convenient to divide the function F into potential parts and "dynamic" parts, through the separation

$$F(\mathbf{R},\mathbf{s})=-Q(\mathbf{R},\mathbf{s})+S(\mathbf{R},\mathbf{s}) . \tag{21}$$

Let us deal with the second term first. In general, the dynamic terms are related to the integral invariants of the motion, and may be written in terms of a sum, as[19]

$$\int^{\beta}F(\mathbf{R},\mathbf{s})d\beta'=-\sum_{k=0}^{n}\mathcal{I}_k\mathcal{P}_k , \tag{22}$$

where $\mathcal{I}_k$ is the integral invariant and $\mathcal{P}_k$ is the conjugate quantum-mechanical operator. The most common application is to let $\mathcal{I}_0$ be β and $\mathcal{P}_0$ be H, the total Hamiltonian, in solving the Schrödinger equation. Here, however, we note that it is the off-diagonal difference variable s that transforms, through a Wigner-Weyl transform, into the equivalent momentum, so that the form will be somewhat different for our application. Yet, it is easy to see that the form we want, which must satisfy limitations upon taking derivatives with respect to s and a subsequent limit in this variable, can be expressed as, for the energy

$$\int^{\beta}S(\mathbf{R},\mathbf{s})d\beta'=J(\mathbf{R},\mathbf{s})=\frac{i\mathbf{p}_d\cdot\mathbf{s}}{\hbar}-\frac{m}{2\beta}\left[\frac{\mathbf{s}}{\hbar}\right]^2-\tfrac{3}{2}\ln(\beta) , \tag{23}$$

which can be achieved by consideration of a "drifted Maxwellian" form for the Wigner function itself (Appendix A). Now, the last term may be considered in light of the first term in (4), reflecting the change in the density normalization with position. This term leads to adding the term $-d/2\beta$ to S, where d is the dimensionality of the system (here taken to be 3). After differentiating with respect to β, we note that the s term is equivalent to the harmonic-oscillator potential, normalized by the temperature, in the transverse coordinate. This is somewhat reassuring in that its form is reminiscent of that used by Feynman and Kleinert[17] and given as the last term of (4). The momentum term of (22) is more problematic, however, since the normal dimensionless form is just $\mathbf{p}_d\cdot\mathbf{s}/\hbar$, which does not involve β, and which will vanish in S. While this satisfies the general requirements of (22), it does not fully allow for the replication that we expect to find in solving the differential equation for quantum potentials, and we will need to treat the approximations that will then be required. Therefore, this term now leads to

$$S(\mathbf{R},\mathbf{s})=\frac{m}{2}\left[\frac{\mathbf{s}}{\hbar\beta}\right]^2-\frac{3}{2\beta} . \tag{24}$$

The variation with the average position $\mathbf{R}$ arises from the slow spatial variation of the integral invariants. If we now introduce these results into (19), we find that

$$\begin{aligned}-Q(\mathbf{R},\mathbf{s})+S(\mathbf{R},\mathbf{s})&=-Q(\mathbf{R},\mathbf{s})+\frac{m\mathbf{s}^2}{2\hbar^2\beta^2}-\frac{3}{2\beta}\\&=\frac{\hbar^2}{8m\rho}\nabla^2\rho+\frac{\hbar^2}{2m\rho}\frac{\partial^2\rho}{\partial \mathbf{s}^2}\\&=\frac{\hbar^2}{8m\rho}\nabla^2\rho-\frac{\hbar^2\beta}{2m}\frac{\partial^2(W+Q)}{\partial \mathbf{s}^2}+\frac{\hbar^2}{2m}\frac{\partial^2 J}{\partial \mathbf{s}^2}+\frac{\hbar^2}{2m}\left[-\beta\frac{\partial(W+Q)}{\partial \mathbf{s}}+\frac{\partial J}{\partial \mathbf{s}}\right]^2 .\end{aligned} \tag{25}$$

Now, using (24) and (25), we can rewrite this as

$$-Q(\mathbf{R},\mathbf{s})=\frac{\hbar^2}{8m\rho}\nabla^2\rho-\frac{\hbar^2\beta}{2m}\frac{\partial^2(W+Q)}{\partial\mathbf{s}^2}+\frac{\hbar^2}{2m}\left[\beta\frac{\partial(W+Q)}{\partial\mathbf{s}}\right]^2-\frac{\hbar^2\beta}{m}\frac{\partial(W+Q)}{\partial\mathbf{s}}\frac{\partial J}{\partial\mathbf{s}}\ . \tag{26}$$

In (26), we have ignored the terms in $\mathbf{p}_d$, since we are more interested in the diffusive nonlocality than the drift-induced nonlocality. We will thus approximate these terms as being small (and similarly in the remaining term in J). We note that the derivative of W with respect to the difference variable $\mathbf{s}$ disappears in the limit of small $\mathbf{s}$. Similarly, we expect that the derivative of the quantum potential Q with respect to $\mathbf{s}$ is also small in this limit. In fact, this is formally true in that these potentials are basically functions of the *magnitude* of the difference variable and are symmetry across the main diagonal of the density matrix. Thus, their derivatives with respect to $\mathbf{s}$ must vanish in the limit that the diagonal is approached. Consequently, we shall invoke an *asymptotic approximation,* in which we assert that our interest is primarily in the limit of small $\mathbf{s}$, so that we shall ignore the nonlinear term (the next to the last term) of (26), as being negligible in the overall result.

We are now left with the quantum potential itself. For this, we note that the derivatives also include the applied potential and therefore require that the replication occurs through the differential equation

$$-\frac{\hbar^2\beta}{2m}\frac{\partial^2(W+Q)}{\partial\mathbf{s}^2}+\mathbf{s}\frac{\partial(W+Q)}{\partial\mathbf{s}}+[Q(\mathbf{R},\mathbf{s})+W(\mathbf{R},\mathbf{s})]=-\frac{\hbar^2}{8m\rho}\nabla^2\rho+W(\mathbf{R},\mathbf{s})\ . \tag{27}$$

We now scale the difference coordinate by the thermal wavelength through the change of variables

$$\mathbf{x}=\frac{\mathbf{s}}{\lambda_D},\quad \lambda_D^2=\frac{\hbar^2\beta}{2m}\ . \tag{28}$$

This leads to the differential equation

$$\frac{\partial^2(W+Q)}{\partial\mathbf{x}^2}-\mathbf{x}\frac{\partial(W+Q)}{\partial\mathbf{x}}-(W+Q)=-U_0\ , \tag{29}$$

where

$$U_0=-\frac{\hbar^2}{8m\rho}\nabla^2\rho+W\ . \tag{30}$$

It is clear now that the total effective potential involves the "quantum potential," which is how we shall discuss the first term in (30), as well as the actual potential, and an effective harmonic-oscillator potential, as suggested in (4) and (5). The potential function W will now be replaced by a nonlocal one, in which the actual potential variation is weighted by the Green's function of the left-hand side of (29), just as in (4). Were it not for the sign of the last term on the left of (29), the solutions would be simply harmonic-oscillator functions, e.g., Hermite polynomials. However, this sign complicates the result, and the solutions are actually parabolic cylinder functions [the factor of 2 added in (28) is just to make the solution easier].

Equation (29) can be solved through the use of a Green's function, which itself must satisfy the adjoint equation[20]

$$\frac{\partial^2 G}{\partial\mathbf{x}^2}+\frac{\partial\mathbf{x}G}{\partial\mathbf{x}}-G=-\delta(\mathbf{x}-\mathbf{x}')\ , \tag{31}$$

under the restriction that both the Green's function and its derivative with respect to $\mathbf{x}$ vanishes at infinity. Then, by the normal tricks, the solution will be found to be (the definition $R=W+Q$ is used)

$$R=\int d\mathbf{x}'U_0(\mathbf{x}')G(\mathbf{x},\mathbf{x}')\ . \tag{32}$$

The task is to find the Green's function itself. In Appendix B, the solution of this equation is shown to be (normalized)

$$G(x)=\frac{1}{4\pi x}e^{-x^2/2}\ , \tag{33}$$

where $x=|\mathbf{x}-\mathbf{x}'|$. This can now be used in (33) to evaluate the nonlocal potential. This equation is the first part of our result, and states that the potentials in the exponent of (20) must be considered as nonlocal quantities. In fact, the effect of the Green's function is to average R over a sphere whose radius is of the order of λ_D. This effectively accounts for the diffusive effects of the potential represented by the nonlocality. Indeed, the three-dimensional integration provides (within numerical factors) precisely the smoothing function of (5) for the Feynman approach. Even when we pass to the limit of $s\rightarrow 0$, we are still left with the result that the various potential terms are smoothed by averaging over a sphere whose radius is approximately the thermal Debye wavelength (the integration over s' goes into an integration over $\mathbf{r}'$). In fact, the key radial integration leads to the weighting, which is zero at the origin and sharply peaked at a radius of approximately 0.58. This means that the actual value of the *effective* potential is that of the potential averaged over a thick *shell* of radius of about $0.82\lambda_D$. Thus, the *effective potential* is constructed by an average of its actual values about λ_D in distance. At high temperatures, this quantity is small and the classical locality is recovered.

Now, we note at this point that the above prescription means that we replace the density term *and* the classical, local potential function with the new nonlocally smoothed function (32). Thus, in the following, the quantity $R=W+U_Q$ refers to the smoothed nonlocal potential. The actual "quantum potential" may be obtained as a part of this total potential, but it should be recognized that the local classical potential no longer even appears in the problem, and is only recovered in the high-temperature limit.

THE HYDRODYNAMIC EQUATIONS

We may now write down the hydrodynamic equations using the results of the preceding section. This is done in the absence of collisions, but these can be easily added in a variety of ways.[7,8,14] The continuity equation is just (12), and we evaluate the momentum through

$$\begin{aligned}\lim_{s\to 0}\left[-i\hbar\frac{\partial\rho}{\partial \mathbf{s}}\right]&=i\hbar\beta\lim_{s\to 0}\left[\frac{\partial(W+Q)}{\partial \mathbf{s}}-\frac{\partial J}{\partial \mathbf{s}}\right]\rho\\&=-i\hbar\beta\lim_{s\to 0}\left[\frac{\partial J}{\partial \mathbf{s}}\right]\rho\\&=\mathbf{p}_d n(\mathbf{R})\ ,\end{aligned} \tag{34}$$

where we have used the asymptotic approximation, in which it is recognized that the function $W+Q$ is symmetric across the diagonal of the density matrix, to eliminate the first term in the square brackets as before, and used J from (23). The continuity equation then becomes

$$\frac{\partial n}{\partial t}+\nabla\cdot[\mathbf{v}_d n(\mathbf{R})]=0\ , \tag{35}$$

where $\mathbf{v}_d=\mathbf{p}_d/m$ is the drift velocity. The only impact of the quantum potential here is in the actual form of the density.

The momentum equation is obtained from the earlier (15). To evaluate this, we need the term

$$\begin{aligned}-\frac{\hbar^2}{2m}\lim_{s\to 0}\frac{\partial^2}{\partial \mathbf{s}^2}\rho&=\lim_{s\to 0}\left\{\frac{\hbar^2}{2m}\left[\beta\frac{\partial^2(W+Q)}{\partial \mathbf{s}^2}-\frac{\partial^2 J}{\partial \mathbf{s}^2}\right]\rho-\frac{\hbar^2}{2m}\left[\beta\frac{\partial(W+Q)}{\partial \mathbf{s}}-\frac{\partial J}{\partial \mathbf{s}}\right]^2\rho\right\}\\&=\lim_{s\to 0}\left\{\left[U_{\text{eff}}+\frac{3}{2\beta}\right]\rho-\frac{1}{2m}\left[i\mathbf{p}_d-\frac{ms}{\hbar\beta}\right]^2\rho\right\}\\&=\left[U_{\text{eff}}+\frac{3}{2\beta}+\frac{\mathbf{p}_d^2}{2m}\right]n(\mathbf{R})\ ,\end{aligned} \tag{36}$$

where we have used (23) in the second line, the asymptotic approximation, and

$$U_{\text{eff}}=\frac{\hbar^2\beta}{2m}\frac{\partial^2(W+Q)}{\partial \mathbf{s}^2}=\frac{\partial^2(W+Q)}{\partial \mathbf{x}^2} \tag{37}$$

defines the *effective potential.* It is this potential which will appear in the hydrodynamic equations, not the smoothed potential that arises in the density matrix itself. Thus, while the density is related to a nonlocal potential, which is a smoothed version of the classical potential and a quantum correction term, the forcing terms in the hydrodynamic equations arise from the effective potential, which is the difference between the actual potential and the smoothed potential. To see this, we use (29), noting that the first derivative term can be ignored since we are interested in the limit as $\mathbf{s}\to 0$, to see that

$$\begin{aligned}U_{\text{eff}}&=\frac{\partial^2(W+Q)}{\partial \mathbf{x}^2}=W+Q-U_0\\&=\lim_{x\to 0}\int d\mathbf{x}'U_0(\mathbf{x}')[G(\mathbf{x},\mathbf{x}')-\delta(\mathbf{x}-\mathbf{x}')]\ .\end{aligned} \tag{38}$$

Then, (11) becomes (recall that we are using the diagonal approximation to the pressure tensor)

$$\frac{\partial}{\partial t}[\mathbf{p}_d n(\mathbf{R})]+\nabla\left\{\left[U_{\text{eff}}+\frac{3}{2\beta}+\frac{\mathbf{p}_d^2}{2m}\right]n(\mathbf{R})\right\}=-\nabla V n(\mathbf{R})\ . \tag{39}$$

This may be combined with the continuity equation (29) to yield the momentum balance equation

$$\frac{\partial \mathbf{p}_d}{\partial t}+\mathbf{v}_d\cdot\nabla\mathbf{p}_d+\frac{1}{n(\mathbf{R})}\nabla\left\{\left[U_{\text{eff}}+\frac{3}{2\beta}\right]n(\mathbf{R})\right\}=-\nabla V\ . \tag{40}$$

Clearly now, the effective potential appears as an added energy or, in keeping with the original understanding of this term, a quantum pressure that adds to the thermal pressure.

To get the energy equation, we need to take the second derivative of (11) with respect to the difference coordinate $\mathbf{s}$, and then pass to the limit of vanishing $\mathbf{s}$. For this, we will need to evaluate the third derivative of the density matrix, with respect to the difference coordinate. In keeping with the previous approximations, we seek the term

$$-\frac{i\hbar^3}{6m^2}\lim_{s\to 0}\frac{\partial^3}{\partial \mathbf{s}^3}\rho\ . \tag{41}$$

Then

$$\begin{aligned}\frac{\partial^3}{\partial \mathbf{s}^3}\rho=&\left[i\frac{\mathbf{p}_d}{\hbar}-\frac{ms}{\hbar^2\beta}\right]^3\rho\\&-3\left[\frac{\beta}{\lambda_D^2}U_{\text{eff}}+\frac{3m}{\hbar^2\beta}\right]\left[i\frac{\mathbf{p}_d}{\hbar}-\frac{ms}{\hbar^2\beta}\right]\rho\ .\end{aligned} \tag{42}$$

Then,

$$\begin{aligned}\frac{i\hbar^3}{6m^2}\lim_{s\to 0}\frac{\partial^3}{\partial \mathbf{s}^3}\rho&=\frac{\mathbf{p}_d^3}{6m^2}n(\mathbf{R})+\frac{\mathbf{p}_d}{m}\left[U_{\text{eff}}+\frac{3}{2\beta}\right]n(\mathbf{R})\\&=\mathbf{v}_d\left\{\frac{p_d^2}{6m}+\left[U_{\text{eff}}+\frac{3}{2\beta}\right]\right\}n(\mathbf{R})\ .\end{aligned} \tag{43}$$

The energy balance equation then becomes

$$\frac{\partial}{\partial t}[\langle \varepsilon \rangle n(\mathbf{R})]+\nabla\cdot\left\{\mathbf{v}_d\left[\frac{p_d^2}{6m}+U_{\text{eff}}+\frac{3}{2\beta}\right]n(\mathbf{R})\right\} = -\mathbf{v}_d\cdot\nabla V n(\mathbf{R}) \ . \quad (44)$$

This can also be combined with (34) and (40) to obtain an equation just for the time development of the average density, which is the term in the large square brackets of (44). This leads to

$$\frac{\partial\langle \varepsilon \rangle}{\partial t}+\mathbf{v}_d\cdot\nabla\langle \varepsilon \rangle-\frac{1}{3mn(\mathbf{R})}\nabla\cdot[\mathbf{v}_d p_d^2 n(\mathbf{R})] = -\mathbf{v}_d\cdot\nabla V \ , \quad (45)$$

with

$$\langle \varepsilon \rangle=\frac{p_d^2}{2m}+U_{\text{eff}}+\frac{3}{2\beta} \ . \quad (46)$$

We need to remark that this particular form of the energy arises from the very simple approximation used to evaluate the third-rank tensor that arises from the derivatives in (42), which is a simple diagonal approximation. A more careful look at the evaluation of these tensor derivatives will yield a different result for the numerical factors, particularly on the first and third terms. Our emphasis here is the effective potential, and the manner in which it appears in the hydrodynamic equations.

DISCUSSION

It appears that the various approximations that have been made to an effective potential through a variational approach[16–18] are supported to various degrees by the derivation of the quantum potential that is given here. However, this potential, which is a nonlocal average of the semiclassical potential, appears only in the variation of the density (or, more properly, the density matrix) with the potential. The hydrodynamic equations contain an additional driving term, which is not the quantum potential used in previous work. Rather, the extra driving terms derive from the *difference* between the nonlocal potential and the actual local value of the potential. In each case, however, there is an added term to the "potential" that arises from the second derivative of the density, and corresponds to the difference between the Bohm potential and the Wigner potential. It must be pointed out, however, that it is the difference between this term and its nonlocal average that appears as a driving term in the hydrodynamic equations. The spatial, nonlocal average smooths the potential contributions over a distance of the order of the thermal de Broglie wavelength $\lambda_D=\sqrt{\hbar^2\beta/2m}$. Thus, at high temperatures, the effective potential appearing in the hydrodynamic equations actually vanishes since the averaged potential differs little from the local potential. At low temperatures, however, significant variations in the density can arise from these effects.

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APPENDIX A

We wish to show in this appendix that the forms of the functions J and S are quite reasonable. The semiclassical phase-space distribution function has its analog in the Wigner distribution function, which is a Fourier transform of the off-diagonal position variable $\mathbf{s}$ into a momentum variable $\mathbf{p}$. We consider then the Wigner distribution function in the form of a quasidrifted Maxwellian, as

$$W(\mathbf{R},\mathbf{p})=\exp\left[-\frac{\beta}{2m}(\mathbf{p}-\mathbf{p}_d)^2\right] , \quad (\text{A1})$$

where $\mathbf{p}_d$ is the drift momentum. The corresponding density matrix is found from the inverse transform as

$$\rho(\mathbf{R},\mathbf{s})=\frac{1}{8\pi^3\hbar^3}\int d^3\mathbf{p}\exp\left[-\frac{\beta}{2m}(\mathbf{p}-\mathbf{p}_d)^2-i\frac{\mathbf{p}\cdot\mathbf{s}}{\hbar}\right] . \quad (\text{A2})$$

The integration over the azimuthal angle can be done immediately, but that over the polar angle (with $\mathbf{s}$ taken to be the polar direction) is slightly more complicated. Nevertheless, it is straightforward, yielding

$$\rho(\mathbf{R},\mathbf{s})=\frac{1}{4\pi^2\hbar^3}\frac{m}{\beta\alpha}\int_{-\infty}^{\infty}p\,dp\exp\left[-\frac{\beta p^2}{2m}-\frac{\beta\alpha}{m}p\right] , \quad (\text{A3})$$

where

$$\alpha=\left|\mathbf{p}_d+\frac{m\mathbf{s}}{\hbar\beta}\right| . \quad (\text{A4})$$

While this latter quantity has been written in this manner for convenience, all of the vector angles will be preserved at the end. Completing the square in the exponent and evaluating the resulting Gaussian integral yields

$$\rho(\mathbf{R},\mathbf{s})=\frac{1}{\sqrt{2\pi}\pi\hbar^3}\left[\frac{m}{\beta}\right]^{3/2}\exp\left[-\frac{\beta}{2m}(\mathbf{p}_d^2-\alpha^2)\right]$$
$$=\left[\frac{m}{2\pi}\right]^{1/2}\frac{m}{\pi\hbar^3}\exp\left[-\frac{m\mathbf{s}^2}{2\hbar^2\beta}+i\frac{\mathbf{p}_d\cdot\mathbf{s}}{\hbar}-\tfrac{3}{2}\ln(\beta)\right] . \quad (\text{A5})$$

This is the form that is used in the text.

APPENDIX B

Our beginning place to compute the Green's function for the quantum potential is (34), which may be rewritten as

$$\frac{\partial^2 G}{\partial\mathbf{x}^2}+\frac{\partial^x G}{\partial\mathbf{x}}-G=-\delta(\mathbf{x}-\mathbf{x}') . \quad (\text{B1})$$

The dot product in the second term on the left assures us of seeking primarily the radial portion of the solution, so that we can approximate the Green's function as a spherically symmetric quantity, and can write it in terms of $x=|\mathbf{x}-\mathbf{x}'|$. Then, Fourier transforming (B1) leads to

$$\left[-k^2-k\frac{\partial}{\partial k}-1\right]G(k)=-1\ . \tag{B2}$$

This, in turn, can be rewritten as

$$k\frac{\partial G}{\partial k}+k\frac{\partial}{\partial k}\left[\frac{k^2}{2}+\ln(k)\right]G=1\ . \tag{B3}$$

We can now solve for the Fourier transform of the Green's function to be

$$G(k)=\sqrt{\pi/2}\frac{1}{ik}e^{-k^2/2}\Phi\left[\frac{k}{i\sqrt{2}}\right]\ , \tag{B4}$$

where $\Phi(x)$ is the error function. The (three-dimensional) inverse Fourier transform of this gives

$$G(x)=\frac{1}{8\sqrt{\pi}x}e^{-x^2/2}\ . \tag{B5}$$

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