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Smooth quantum potential for the hydrodynamic model

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An effective stress tensor and energy density for the quantum hydrodynamic (QHD) equations are derived in the Born approximation to the Bloch equation. The quantum potential appearing in the stress tensor and energy density is valid to all orders of $\hbar^2$ and to first order in βV, and involves both a smoothing integration of the classical potential over space and an averaging integration over temperature. In the presence of discontinuities in the classical potential (which occur, for example, at potential barriers in semiconductors), the effective stress tensor and energy density are more tractable analytically and numerically than in the original $O(\hbar^2)$ QHD theory. By cancelling the leading singularity in the classical potential at a barrier and leaving a residual smooth effective potential (with a lower potential height) in the barrier region, the effective stress tensor makes the barrier partially transparent to the particle flow and provides the mechanism for particle tunneling in the QHD model.

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I. INTRODUCTION

Quantum systems can be described under certain circumstances by classical equations in which the classical potential energy is replaced by an effective potential incorporating quantum effects. The quantum potential of Madelung and Bohm for the hydrodynamic formulation of (pure state) quantum mechanics [1,2], the $O(\hbar^2)$ Wigner distribution function [3], and the effective classical partition function of Feynman and Kleinert [4] are famous examples of this strategy, which play a role in formulating quantum hydrodynamics.

Important quantum effects in compressible fluids— for example, electrons tunneling through a potential barrier in a semiconductor—can be described near thermal equilibrium and in the high-temperature limit by quantum hydrodynamic (QHD) equations (see [5] and references therein), which have the same form as the classical hydrodynamic equations (the Euler equations of gas dynamics). Quantum terms appear in the equations of gas dynamics in the expression for the stress tensor and in the energy density derived from the stress tensor, rather than in the potential energy terms.

Originally the quantum correction to the stress tensor in the QHD equations was given to $O(\hbar^2)$ [the actual expansion parameter is $\hbar^2/8mTl^2$, where l is a characteristic length scale in the problem; we will use the shorthand $O(\hbar^2)$], and involved second derivatives of the classical potential (which is discontinuous at a potential barrier). The derivation of the QHD equations assumed that the classical potential has a Taylor series expansion. In the spirit of Feynman and Kleinert, Ferry and Zhou derived a "form" for a smooth quantum potential [6] for the QHD equations by linearizing an equation for the equilibrium density matrix. The Feynman-Kleinert effective partition function (see Appendix A for details) involves a smoothed potential of the form

$$V_{a^2}(x)=\int \frac{dy}{\sqrt{2\pi a^2}}\exp\left\{-\frac{(x-y)^2}{2a^2}\right\}V(y)\ , \qquad (1)$$

where V is the classical potential energy, $a^2\propto\beta\hbar^2/m$, $\beta=1/T$ is the inverse temperature (we set Boltzmann's constant $k_B=1$), and m is the particle mass. The Ferry-Zhou effective stress tensor involves the difference between the smoothed and the local quantum potential $-\hbar^2\nabla^2 n/8mn+V$, where n is the particle density. Their smoothing function is of the form $\exp\{-(\mathbf{x}-\mathbf{y})^2/2a^2\}/|\mathbf{x}-\mathbf{y}|$. Note that the off-diagonal entries in the stress tensor are neglected in [6].

This investigation extends the analysis of the quantum potential by first deriving an expression for the effective equilibrium density matrix from the Bloch equation in the Born approximation. Then the QHD equations including the effective stress tensor and the effective energy density are calculated using the density matrix in a moment expansion of the quantum Liouville equation. As $\hbar\to 0$, the extended QHD equations reproduce the original $O(\hbar^2)$ equations, yet their derivation does not require the classical potential to have a Taylor series expansion.

The effective density matrix has the form

$$\rho(\beta,\mathbf{x},\mathbf{y})\approx\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\times\exp\left\{-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{y})^2-\beta\tilde{V}(\beta,\mathbf{x},\mathbf{y})\right\}\ , \qquad (2)$$

where $\tilde{V}$ is given by Eq. (25). The density matrix is the Fourier transform of the Wigner distribution function f_W:

$$\rho(\mathbf{x},\mathbf{y})=\int d^3p\, f_W\left[\frac{\mathbf{x}+\mathbf{y}}{2},\mathbf{p}\right]e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})/\hbar}\ , \qquad (3)$$

where $\mathbf{p}$ is the momentum. If f_W is set equal to the classical Maxwell-Boltzmann distribution function $e^{-\beta E}/(2\pi\hbar)^3$ where $E=p^2/2m+V$, we obtain the "classical" density matrix

$$\rho_C(\beta,\mathbf{x},\mathbf{y})=\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\times\exp\left\{-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{y})^2-\beta V\left[\frac{\mathbf{x}+\mathbf{y}}{2}\right]\right\}. \tag{4}$$

[The classical density matrix satisfies the $\hbar\to 0$ limit of the Bloch equation (8).] The effective density matrix (2) is obtained from ρ_C by replacing $V[(\mathbf{x}+\mathbf{y})/2]$ with $\bar{V}(\beta,\mathbf{x},\mathbf{y})$.

The quantum correction to the classical stress tensor is valid to all orders of $\hbar^2$ and to first order in $\beta\delta V$, where $\delta V\equiv\max\{V\}-\min\{V\}$ over a characteristic length scale, and involves both a smoothing integration of the classical potential over space and an averaging integration over temperature. The effective stress tensor is given in the Born approximation by

$$P_{ij}=-nT\delta_{ij}-\frac{\hbar^2 n}{4mT}\frac{\partial^2\bar{V}}{\partial x_i\partial x_j}, \tag{5}$$

where the "quantum potential" is

$$\bar{V}(\beta,\mathbf{x})=\frac{1}{\beta}\int_0^\beta d\beta'\left[\frac{\beta'}{\beta}\right]^2\int d^3X'\left[\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right]^{3/2}\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}(\mathbf{X}'-\mathbf{x})^2\right\}V(\mathbf{X}'). \tag{6}$$

Note that changing the classical potential V by an effective constant does not change the effective stress tensor. Thus in constructing the effective stress tensor in the Born approximation, it is the change $\beta\delta V$ over a characteristic length scale that is assumed small rather than βV.

The change $\beta\delta V$ over a characteristic length scale may not be small at a potential step. In fact, for a 0.2-eV barrier, $\beta\delta V\approx 8$ at 300 K and ≈ 32 at 77 K. However, for applications like the resonant tunneling diode, $\beta\delta V\ll 1$ except at the potential jumps. In addition, numerical comparisons [7] demonstrate excellent agreement between the first three moments (the second moment vanishes) of the equilibrium full density matrix and the effective density matrix for the Bloch equation with a double barrier potential for $\beta\delta V\lesssim 1$, and good qualitative agreement for $\beta\delta V\lesssim 20$. The moments of the $O(\hbar^2)$ density matrix are in severe quantitative and qualitative disagreement with the moments of the full density matrix. For classical potentials with discontinuities, the extended QHD solution will always be more accurate than the $O(\hbar^2)$ QHD solution, since the $O(\hbar^2)$ QHD equations involve third derivatives of the potential discontinuities.

The stress tensor and energy density display the nonlocal character of quantum mechanics since P_{ij} depends through the derivatives $\partial^2/\partial x_i\partial x_j$ on the quantum potential not only at $\mathbf{x}$ but in a neighborhood of $\mathbf{x}$. In addition, the quantum potential (6) involves a nonlocal Gaussian-weighted smoothing of the classical potential. Through the second derivatives of the quantum potential, particles experience a force[4] due to the classical potential averaged over a ball of radius equal to a few times $\sqrt{\beta\hbar^2/4m}$. For electron propagation in GaAs, this radius is approximately 70 Å at 77 K (liquid-nitrogen temperature) and 35 Å at 300 K. Classical mechanics is recovered as $T\to\infty$, since $\bar{V}\to V/3$ and $P_{ij}\to -nT\delta_{ij}$.

The thermal averaging $\int_0^\beta d\beta'\beta'^2$ gives rise to a statistical factor of $\frac{1}{3}$ when the quantum potential is expanded to leading order in $\hbar^2$: $\bar{V}(\beta,\mathbf{x})=V(\mathbf{x})/3+O(\hbar^2)$. Using this approximation in Eq. (5) reproduces the $O(\hbar^2)$ stress tensor

$$P_{ij}^{(2)}=-nT\delta_{ij}-\frac{\hbar^2 n}{12mT}\frac{\partial^2 V}{\partial x_i\partial x_j}. \tag{7}$$

The expression (7) for P_{ij} introduces *third* derivatives of the classical potential into the hydrodynamic equations. In general V may have discontinuities, and the third derivatives of V present both analytical and computational problems. Our goal here is to rigorously justify the smooth effective stress tensor (5), which has the same smoothness properties as the classical potential.

The effective stress tensor actually cancels the leading singularity in the classical potential at a barrier (see Figs. 1 and 2 and Sec. IV) and leaves a residual smooth effective potential (with a lower potential height) in the barrier region. This cancellation and smoothing makes the barrier partially transparent to the particle flow and provides the mechanism for particle tunneling in the QHD model. Note that the effective potential in Fig. 1 produces a repulsive force near the barrier edges that is stronger as $T\to\infty$ and extends for roughly [75 (Å)]$\times\sqrt{[300\text{ (K)}]/T}$. The barrier height in Fig. 2 approaches zero as $T\to 0$. These effects provide a fluid dynamical explanation of why particle tunneling is enhanced at low temperatures. As $T\to\infty$, the effective potential approaches the classical barrier potential and quantum effects in the QHD model are suppressed.

In our derivation of the extended QHD equations, we follow the basic approach of Ferry and Zhou. Our approach differs from theirs in that we (1) explicitly calcu-

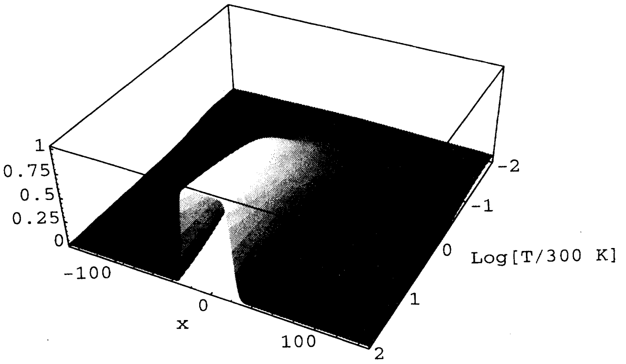

FIG. 1. Smooth effective potential for electrons in GaAs for a 50-Å-wide unit potential barrier as a function of x in Å and $\log_{10}\{T/[300\ (\mathrm{K})]\}$ for $3 \leq T \leq 30\,000$ K.

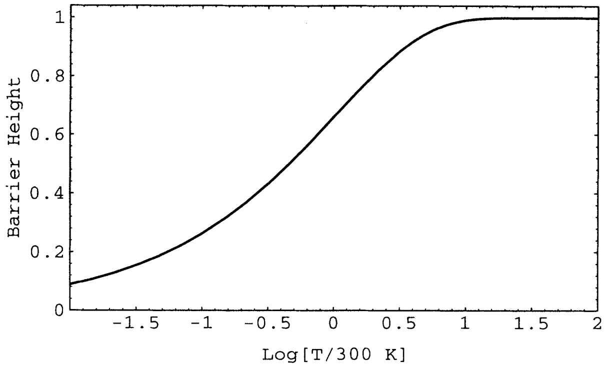

FIG. 2. Maximum barrier height (at $x=0$) of the smooth effective potential in Fig. 1.

late the effective density matrix, (2) evaluate the full effective stress tensor including the off-diagonal elements, and (3) use a Green's function method and the Born approximation for solving the Bloch equation. Our new effective stress tensor for the QHD equations involves a quantum potential that is given explicitly in terms of the classical potential and introduces an averaging over temperature in addition to the smoothing integration over space.

The effective density matrix valid to all orders of $\hbar^2$ and to first order in $\beta\delta V$ is calculated in Sec. II. Section III gives the derivation of the QHD equations (including the effective stress tensor and energy density) from the effective density matrix. In Sec. IV we discuss the smoothness and cancellation properties of the effective stress tensor and energy density, and give the jump relations for the extended QHD equations at a potential discontinuity. Finally Appendix A presents the relationship between the Feynman-Kleinert partition function and the $O(\hbar^2)$ Wigner distribution function, and Appendix B shows that the effective density matrix when expanded to $O(\hbar^2)$ agrees with Wigner's $O(\hbar^2)$ density matrix.

II. THE EFFECTIVE DENSITY MATRIX

In thermal equilibrium, the density matrix satisfies the Bloch equation

$$\frac{\partial\rho}{\partial\beta} = -\frac{1}{2}(H_x+H_y)\rho = \frac{\hbar^2}{4m}(\nabla_x^2+\nabla_y^2)\rho - \frac{1}{2}[V(\mathbf{x})+V(\mathbf{y})]\rho \ , \tag{8}$$

where the Hamiltonian $H_x = -\hbar^2\nabla_x^2/2m + V(\mathbf{x})$ and where we have assumed Boltzmann statistics. We will solve the Bloch equation for the effective density matrix in the Born approximation using a Green's function method.

The reason we start with the Bloch equation is that steady-state solutions of the quantum Liouville equation (26) need not be thermal equilibrium solutions; i.e., they may not satisfy the Bloch equation. On the other hand, solutions $\rho_B(\beta,\mathbf{x},\mathbf{y})$ of the Bloch equation are solutions of the time-independent quantum Liouville equation without scattering (the Heisenberg equation)

$$(H_x - H_y)\rho = 0 \tag{9}$$

if $\rho_B(\beta=0,\mathbf{x},\mathbf{y})$ is a solution of Eq. (9). To see this, define $\rho_L = (H_x - H_y)\rho_B$. Then

$$\begin{aligned}\frac{\partial\rho_L}{\partial\beta} &= -\frac{1}{2}(H_x-H_y)(H_x+H_y)\rho_B \\ &= -\frac{1}{2}(H_x+H_y)(H_x-H_y)\rho_B \\ &= -\frac{1}{2}(H_x+H_y)\rho_L \ .\end{aligned} \tag{10}$$

Thus if $\rho_L(\beta=0,\mathbf{x},\mathbf{y})=0$, $\rho_L(\beta,\mathbf{x},\mathbf{y})$ remains zero for all β and ρ_B is a solution of the Heisenberg equation. The effective density matrix (2) equals $\delta^{(3)}(\mathbf{x}-\mathbf{y})$ as $\beta\to 0$, which is a $\beta=0$ solution of the Heisenberg equation. Therefore the effective density matrix, which is an $O(\beta\delta V)$ solution of the Bloch equation, is guaranteed to be an $O(\beta\delta V)$ solution of the Heisenberg equation for all β. To derive the fluid dynamical equations as moments of the quantum Liouville equation, we then allow the parameters in the effective density matrix to vary slowly in space and time.

The Green's function for the Bloch equation can be written down from the Green's function for the six-dimensional (6D) heat equation:

$$G(\beta,\mathbf{x},\mathbf{y};\beta',\mathbf{x}',\mathbf{y}') = \left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3 \exp\left\{-\frac{m}{(\beta-\beta')\hbar^2}[(\mathbf{x}-\mathbf{x}')^2+(\mathbf{y}-\mathbf{y}')^2]\right\}\theta(\beta-\beta') \ , \tag{11}$$

where θ is the unit step function. Then the Green's function solution to the Bloch equation is

$$\rho(\beta,\mathbf{x},\mathbf{y})=\int d^3x'\,d^3y'\,G(\beta,\mathbf{x},\mathbf{y};0,\mathbf{x}',\mathbf{y}')\rho(0,\mathbf{x}',\mathbf{y}')-\tfrac{1}{2}\int_0^{\beta}d\beta'\int d^3x'\,d^3y'\,G(\beta,\mathbf{x},\mathbf{y};\beta',\mathbf{x}',\mathbf{y}')[V(\mathbf{x}')+V(\mathbf{y}')]\rho(\beta',\mathbf{x}',\mathbf{y}')\ , \tag{12}$$

where the initial condition is $\rho(0,\mathbf{x},\mathbf{y})=\delta^{(3)}(\mathbf{x}-\mathbf{y})$. Using this initial condition and the Green's function (11), we obtain

$$\rho(\beta,\mathbf{x},\mathbf{y})=\rho_0(\beta,\mathbf{x},\mathbf{y})-\frac{1}{2}\int_0^{\beta}d\beta'\int d^3x'\,d^3y'\left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3 \times\exp\left\{-\frac{m}{(\beta-\beta')\hbar^2}[(\mathbf{x}-\mathbf{x}')^2+(\mathbf{y}-\mathbf{y}')^2]\right\}[V(\mathbf{x}')+V(\mathbf{y}')]\rho(\beta',\mathbf{x}',\mathbf{y})\ , \tag{13}$$

where the free-particle ($V=0$) density matrix is

$$\rho_0(\beta,\mathbf{x},\mathbf{y})=\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\exp\left\{-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{y})^2\right\}\ . \tag{14}$$

Next we solve Eq. (13) iteratively. We set $\rho=\rho_0$ inside the integral to get the first approximation (Born approximation) ρ_1 to ρ:

$$\begin{aligned}\rho(\beta,\mathbf{x},\mathbf{y})&\approx\rho_1(\beta,\mathbf{x},\mathbf{y})\\ &=\rho_0(\beta,\mathbf{x},\mathbf{y})-\frac{1}{2}\int_0^{\beta}d\beta'\int d^3x'\,d^3y'\left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3\left[\frac{m}{2\pi\beta'\hbar^2}\right]^{3/2}\\ &\qquad\times\exp\left\{-\frac{m}{(\beta-\beta')\hbar^2}[(\mathbf{x}-\mathbf{x}')^2+(\mathbf{y}-\mathbf{y}')^2]-\frac{m}{2\beta'\hbar^2}(\mathbf{x}-\mathbf{y}')^2\right\}[V(\mathbf{x}')+V(\mathbf{y}')]\ .\end{aligned} \tag{15}$$

The Gaussian inside the integral is maximum at $\mathbf{x}'=\mathbf{x}_0$, $\mathbf{y}'=\mathbf{y}_0$ where

$$\mathbf{x}_0=\frac{1}{2}\left[1+\frac{\beta'}{\beta}\right]\mathbf{x}+\frac{1}{2}\left[1-\frac{\beta'}{\beta}\right]\mathbf{y}\ , \tag{16}$$

$$\mathbf{y}_0=\frac{1}{2}\left[1-\frac{\beta'}{\beta}\right]\mathbf{x}+\frac{1}{2}\left[1+\frac{\beta'}{\beta}\right]\mathbf{y}\ . \tag{17}$$

Expanding the exponent in the Gaussian about $\mathbf{x}'=\mathbf{x}_0$, $\mathbf{y}'=\mathbf{y}_0$, we obtain

$$\rho(\beta,\mathbf{x},\mathbf{y})\approx\rho_1(\beta,\mathbf{x},\mathbf{y})=\rho_0(\beta,\mathbf{x},\mathbf{y})[1-\beta\tilde{V}(\beta,\mathbf{x},\mathbf{y})]\approx\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\exp\left\{-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{y})^2-\beta\tilde{V}(\beta,\mathbf{x},\mathbf{y})\right\}\ , \tag{18}$$

where the "6D quantum potential" is

$$\begin{aligned}\tilde{V}(\beta,\mathbf{x},\mathbf{y})&=\frac{1}{2\beta}\int_0^{\beta}d\beta'\int d^3x'\,d^3y'\left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3\left[\frac{\beta}{\beta'}\right]^{3/2}\\ &\qquad\times\exp\left\{-\frac{m}{2\beta'\hbar^2}\frac{\beta+\beta'}{\beta-\beta'}\left[(\mathbf{x}'-\mathbf{x}_0)^2-2\frac{\beta-\beta'}{\beta+\beta'}(\mathbf{x}'-\mathbf{x}_0)\cdot(\mathbf{y}'-\mathbf{y}_0)+(\mathbf{y}'-\mathbf{y}_0)^2\right]\right\}[V(\mathbf{x}')+V(\mathbf{y}')]\ .\end{aligned} \tag{19}$$

Since the calculation of the stress tensor is most easily accomplished in center-of-mass coordinates, we make the change of variables:

$$\mathbf{R}=\tfrac{1}{2}(\mathbf{x}+\mathbf{y}),\quad \mathbf{s}=\mathbf{x}-\mathbf{y}\ . \tag{20}$$

Note that in terms of the new coordinates

$$\mathbf{x}_0=\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s},\quad \mathbf{y}_0=\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s} \tag{21}$$

and that these new coordinates diagonalize the exponent of the Gaussian in the 6D quantum potential (19):

$$\tilde{V}(\beta,\mathbf{R},\mathbf{s})=\frac{1}{2\beta}\int_0^{\beta}d\beta'\int d^3R'\,d^3s'\left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3\left[\frac{\beta}{\beta'}\right]^{3/2}$$
$$\times\exp\left\{-\frac{2m}{(\beta-\beta')\hbar^2}(\mathbf{R}'-\mathbf{R})^2-\frac{m}{2\hbar^2}\frac{\beta}{\beta'(\beta-\beta')}\left[\mathbf{s}'-\frac{\beta'}{\beta}\mathbf{s}\right]^2\right\}\left[V\left[\mathbf{R}'+\frac{\mathbf{s}'}{2}\right]+V\left[\mathbf{R}'-\frac{\mathbf{s}'}{2}\right]\right]. \tag{22}$$

The expression for the 6D quantum potential can be simplified. First shift $\mathbf{R}'$ and $\mathbf{s}'$ in Eq. (22):

$$\tilde{V}(\beta,\mathbf{R},\mathbf{s})=\frac{1}{2\beta}\int_0^{\beta}d\beta'\int d^3R'\,d^3s'\left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3\left[\frac{\beta}{\beta'}\right]^{3/2}\exp\left\{-\frac{2m}{(\beta-\beta')\hbar^2}R'^2-\frac{m}{2\hbar^2}\frac{\beta}{\beta'(\beta-\beta')}s'^2\right\}$$
$$\times\left[V\left[\mathbf{R}'+\frac{\mathbf{s}'}{2}+\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s}\right]+V\left[\mathbf{R}'+\frac{\mathbf{s}'}{2}+\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s}\right]\right], \tag{23}$$

where in the second potential term we have replaced $\mathbf{s}'$ by $-\mathbf{s}'$. Then we can integrate over one set of coordinates by setting

$$\mathbf{X}'=\mathbf{R}'+\frac{\mathbf{s}'}{2},\quad \mathbf{Y}'=\mathbf{R}'-\frac{\beta}{2\beta'}\mathbf{s}'\ . \tag{24}$$

We obtain

$$\tilde{V}(\beta,\mathbf{R},\mathbf{s})=\frac{1}{2\beta}\int_0^{\beta}d\beta'\int d^3X'\left[\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right]^{3/2}$$
$$\times\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}X'^2\right\}\left[V\left[\mathbf{X}'+\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s}\right]+V\left[\mathbf{X}'+\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s}\right]\right]. \tag{25}$$

III. THE QHD EQUATIONS AND THE QUANTUM POTENTIAL

Quantum hydrodynamic equations may be derived as a moment expansion either of the Wigner-Boltzmann equation using the Wigner distribution function (see, e.g., [5]) or of the quantum Liouville equation using the density matrix (see, e.g., [8] and [6]).

The moment expansion of the Wigner-Boltzmann equation involves integrating powers of p_j (1, p_j, and $p^2/2m$, respectively) against $f_W(\mathbf{x},\mathbf{p})$ in the Wigner-Boltzmann equation to obtain conservation laws for particle number, momentum, and energy.

Here we will derive the QHD equations in the framework of the quantum Liouville equation

$$i\hbar\frac{\partial\rho}{\partial t}+\frac{\hbar^2}{m}\nabla_R\cdot\nabla_s\rho=\left[V\left[\mathbf{R}+\frac{\mathbf{s}}{2}\right]-V\left[\mathbf{R}-\frac{\mathbf{s}}{2}\right]\right]\rho$$
$$-\frac{1}{\tau}\mathbf{s}\cdot\nabla_s\rho-\frac{mT_0}{\hbar^2\tau}s^2\rho\ . \tag{26}$$

Scattering is modeled in Eq. (26) by Fokker-Planck terms (the last two terms on the right-hand side) in order to produce relaxation time scattering terms in the QHD conservation laws (43) and (44) for momentum and energy [8]. The constants multiplying the Fokker-Planck terms yield the relaxation times $\tau_p=\tau$ and $\tau_w=\tau/2$ in the QHD equations. In general, though, τ_w will not have any simple relationship to τ_p.

In the Wigner-Boltzmann framework, the average value of a function $\chi(\mathbf{p})$ equals

$$\langle x\rangle=\int d^3p\,\chi(\mathbf{p})f_W(\mathbf{x},\mathbf{p}) \tag{27}$$

in exact analogy with the average value in classical statistical mechanics using the classical distribution function. In the framework of the Liouville equation, the average value becomes

$$\langle\chi\rangle=\lim_{\mathbf{s}\to 0}\chi\left[\frac{\hbar}{i}\nabla_s\right]\rho(\mathbf{R},\mathbf{s})\ , \tag{28}$$

which can be verified using Eq. (3) in center-of-mass coordinates:

$$\rho(\mathbf{R},\mathbf{s})=\int d^3p\,f_W(\mathbf{R},\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}\ . \tag{29}$$

To derive the hydrodynamic equations we will multiply the effective density matrix by a slowly varying function $\mathcal{A}$ of $\mathbf{R}$ and t:

$$\rho(\beta,\mathbf{R},\mathbf{s})\approx\mathcal{A}(\mathbf{R},t)\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}$$
$$\times\exp\left\{-\frac{m}{2\beta\hbar^2}s^2-\beta\tilde{V}(\beta,\mathbf{R},\mathbf{s})\right\}, \tag{30}$$

with $\tilde{V}$ given by Eq. (25). In the density matrix formalism the particle density $n(\mathbf{x},t)$ is given as

$$n(\mathbf{x},t)=\langle 1\rangle=\lim_{\mathbf{s}\to 0}\rho(\beta,\mathbf{R},\mathbf{s})$$

$$\approx\mathcal{A}\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\exp\{-\beta\bar{V}_0(\beta,\mathbf{x})\} \qquad (31)$$

where

$$\bar{V}_0(\beta,\mathbf{x})=\frac{1}{\beta}\int_0^\beta d\beta'\int d^3X'\left[\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right]^{3/2}$$

$$\times\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}(\mathbf{X}'-\mathbf{x})^2\right\}V(\mathbf{X}') . \qquad (32)$$

The factor $\mathcal{A}$ provides the extra parameter needed to set the total number of particles $\int d^3x\, n(\mathbf{x},t)$ equal to a specified integer M.

The moment expansion of the Liouville equation is obtained by multiplying the Liouville equation with powers of $\hbar\nabla_s/i$ (1, $\hbar\nabla_s/i$, and $-\hbar^2\nabla_s^2/2m$, respectively) and taking the limit $\mathbf{s}\to 0$ to obtain conservation laws for particle number, momentum, and energy:

$$\frac{\partial n}{\partial t}+\frac{1}{m}\frac{\partial\langle p_i\rangle}{\partial x_i}=0 , \qquad (33)$$

$$\frac{\partial\langle p_j\rangle}{\partial t}+\frac{\partial}{\partial x_i}\left\langle\frac{p_ip_j}{m}\right\rangle=-n\frac{\partial V}{\partial x_j}-\frac{\langle p_j\rangle}{\tau} , \qquad (34)$$

$$\frac{\partial}{\partial t}\left\langle\frac{p^2}{2m}\right\rangle+\frac{\partial}{\partial x_i}\left\langle\frac{p_ip^2}{2m^2}\right\rangle$$

$$=-\frac{\langle p_i\rangle}{m}\frac{\partial V}{\partial x_i}-\frac{\langle p^2/2m\rangle-\frac{3}{2}nT_0}{\tau/2} , \qquad (35)$$

where repeated indices are summed over. Thus the quantum hydrodynamic conservation laws have exactly the same form as their classical counterparts. Factors of $\hbar$ appear explicitly only at the fourth and higher moments.

The standard approach to calculating the average values in the moment equations is to use the momentum-shifted version of the effective distribution function or density matrix. The microscopic molecular momentum $\mathbf{p}$ can be expanded about the macroscopic fluid velocity $\mathbf{u}$ as

$$\mathbf{p}=m\mathbf{u}+\mathbf{p}' . \qquad (36)$$

The momentum-shifted Wigner distribution function is then given by replacing $f_W(\mathbf{R},\mathbf{p})$ by $f_W(\mathbf{R},\mathbf{p}')$. The momentum-shifted density matrix is obtained by replacing $\rho(\mathbf{R},\mathbf{s})$ by $e^{im\mathbf{u}\cdot\mathbf{s}/\hbar}\rho(\mathbf{R},\mathbf{s})$ since

$$\int d^3p f_W(\mathbf{R},\mathbf{p}')e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}=e^{im\mathbf{u}\cdot\mathbf{s}/\hbar}\int d^3p' f_W(\mathbf{R},\mathbf{p}')e^{i\mathbf{p}'\cdot\mathbf{s}/\hbar}$$

$$=e^{im\mathbf{u}\cdot\mathbf{s}/\hbar}\rho(\mathbf{R},s) . \qquad (37)$$

We now assume that the momentum-shifted effective density matrix approximates the actual density matrix well enough for the average values in Eqs. (33)–(35) to approximate the actual values. We note that the shifted effective density matrix has five free parameters corresponding to the five unknowns in the hydrodynamic equations (42)–(44): $\mathbf{u}$, $1/\beta=T$, and $\mathcal{A}$, which is proportional to n.

Using the shifted effective density matrix, we obtain

$$\langle p_i\rangle=mnu_i , \qquad (38)$$

$$\left\langle\frac{p_ip_j}{m}\right\rangle=mnu_iu_j-P_{ij},\quad P_{ij}\equiv-\left\langle\frac{p_i'p_j'}{m}\right\rangle , \qquad (39)$$

$$\left\langle\frac{p^2}{2m}\right\rangle\equiv W,\quad W=\frac{1}{2}mnu^2+\left\langle\frac{p'^2}{2m}\right\rangle , \qquad (40)$$

$$\left\langle\frac{p_ip^2}{2m^2}\right\rangle=u_iW-u_jP_{ij}+q_i,\quad q_i\equiv\left\langle\frac{p_i'p'^2}{2m^2}\right\rangle , \qquad (41)$$

where W is the energy density. We have allowed a heat flux term $\mathbf{q}$ in the energy conservation equation, even though it vanishes for our effective density matrix, since heat conduction plays a quantitative role in electron and hole propagation in actual semiconductor derives. The definitions in Eqs. (38)–(41) in terms of average values have the same form as the classical definitions in terms of the Boltzmann distribution function.

Substituting the expressions (38)–(41) into the moment equations (33)–(35), we derive the QHD equations

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x_i}(nu_i)=0 , \qquad (42)$$

$$\frac{\partial}{\partial t}(mnu_j)+\frac{\partial}{\partial x_i}(mnu_iu_j-P_{ij})=-n\frac{\partial V}{\partial x_j}-\frac{mnu_j}{\tau_p} , \qquad (43)$$

$$\frac{\partial W}{\partial t}+\frac{\partial}{\partial x_i}(u_iW-u_jP_{ij}+q_i)=-nu_i\frac{\partial V}{\partial x_i}-\frac{W-\frac{3}{2}nT_0}{\tau_w} . \qquad (44)$$

Finally to calculate P_{ij} and W, first observe that $\langle\chi(\mathbf{p}')\rangle$ with the shifted density matrix is equal to $\langle\chi(\mathbf{p})\rangle_{\text{unshifted}}$ with the unshifted density matrix ρ. Then (using the unshifted ρ) we obtain from Eqs. (30) and (25)

$$P_{ij}=\lim_{\mathbf{s}\to 0}\frac{\hbar^2}{m}\frac{\partial^2\rho}{\partial s_i\partial s_j}\approx-nT\delta_{ij}-\frac{\hbar^2 n}{4mT}\frac{\partial^2\bar{V}}{\partial x_i\partial x_j} , \qquad (45)$$

$$W=\frac{1}{2}mnu^2-\lim_{\mathbf{s}\to 0}\frac{\hbar^2}{2m}\nabla_s^2\rho$$

$$\approx\frac{3}{2}nT+\frac{1}{2}mnu^2+\frac{\hbar^2 n}{8mT}\nabla^2\bar{V} , \qquad (46)$$

where the approximation involved is the Born approximation and where the "quantum potential" is

$$\bar{V}(\beta,\mathbf{x})=\frac{1}{\beta}\int_0^\beta d\beta'\left[\frac{\beta'}{\beta}\right]^2\int d^3X'\left[\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right]^{3/2}\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}(\mathbf{X}'-\mathbf{x})^2\right\}V(\mathbf{X}') . \qquad (47)$$

The reader may verify that the moment derivation yields the classical hydrodynamic equations (classical gas dynamics) if the classical density matrix ρ_C in Eq. (4) is substituted for the effective density matrix.

The Gaussian in Eq. (47) is peaked at $\mathbf{X}'=\mathbf{x}$ with a maximum width $a=\sqrt{\beta\hbar^2/4m}$. In the high-temperature limit ($\beta\rightarrow 0$), the width of the Gaussian goes to zero. For numerical implementation, the formula (47) may be written as

$$\bar{V}(\beta,\mathbf{x})=\int_0^1 d\beta'\,\beta'^2\int\frac{d^3X'}{\pi^{3/2}}\exp\{-X'^2\}\times V\left[\mathbf{x}+\left[\frac{\beta(1-\beta'^2)\hbar^2}{2m}\right]^{1/2}\mathbf{X}'\right]. \tag{48}$$

To recover the $O(\hbar^2)$ theory, expand $V(\mathbf{X}'+\mathbf{x})$ about $\mathbf{x}$ in the quantum potential (47) and integrate. We obtain

$$\bar{V}(\beta,\mathbf{x})=\frac{1}{3}V(\mathbf{x})+\frac{\hbar^2\beta}{30m}\nabla^2V(\mathbf{x})+O(\hbar^4)\ . \tag{49}$$

From Eq. (45) the stress tensor is (to first order in $\beta\delta V$)

$$P_{ij}=-nT\delta_{ij}-\frac{\hbar^2 n}{12mT}\frac{\partial^2 V}{\partial x_i\partial x_j}-\frac{\hbar^4 n}{120m^2T^2}\frac{\partial^4 V}{\partial x_i\partial x_j\partial x_k^2}+O(\hbar^6)\ , \tag{50}$$

which reproduces the $O(\hbar^2)$ expression (7) for $P_{ij}^{(2)}$.

Since $P_{ij}^{(2)}$ contains second derivatives of the classical potential, the stress tensor was written in the original $O(\hbar^2)$ QHD theory as

$$P_{ij}^{(2)}=-nT\delta_{ij}+\frac{\hbar^2 n}{12m}\frac{\partial^2}{\partial x_i\partial x_j}\ln(n) \tag{51}$$

using

$$\frac{\partial}{\partial x_i}\ln(n)\approx-\beta\frac{\partial V}{\partial x_i}+O(\hbar^2)\ . \tag{52}$$

Equation (52) is to leading order in $\hbar^2$ equivalent to the classical thermal equilibrium expression $n\propto\exp(-\beta V)$, and should be approximately valid for very slowly varying n, $\mathbf{u}$, and T. However, note that in the extended QHD theory, the stress tensor (45) involves the quantum potential $\bar{V}$, while the density (31) involves $\bar{V}_0$. Replacing $3\bar{V}$ with $\bar{V}_0$ in Eq. (45) makes an $O(\hbar^4)$ error in P_{ij} since

$$3\bar{V}-\bar{V}_0\approx\frac{\hbar^2\beta}{15m}\nabla^2V\ , \tag{53}$$

which would reduce the validity of the extended QHD theory to $O(\hbar^2)$.

The "hydrodynamic" formulation [1] of pure state quantum mechanics consists of a current continuity equation and a momentum equation:

$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{u})=0\ , \tag{54}$$

$$m\left\{\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right\}=-\nabla(V+Q)\ , \tag{55}$$

where the quantum potential is defined by

$$Q=-\frac{\hbar^2}{2m}\frac{1}{\sqrt{n}}\nabla^2\sqrt{n}\ . \tag{56}$$

The momentum equation (55) can be rewritten as a momentum conservation law analogous to the QHD momentum conservation law (43) with T set equal to zero for the pure state and with the scattering term omitted:

$$\frac{\partial}{\partial t}(mnu_j)+\frac{\partial}{\partial x_i}(mnu_iu_j-P_{ij}^{PS})=-n\frac{\partial V}{\partial x_j} \tag{57}$$

where the (exact) stress tensor for the pure state is

$$P_{ij}^{PS}=\frac{\hbar^2 n}{4m}\frac{\partial^2}{\partial x_i\partial x_j}\ln(n)\ . \tag{58}$$

As noted in the Introduction, the smooth quantum potential (6) provides an explanation (through the thermal averaging $\int_0^\beta d\beta'\beta'^2$) of the statistical factor $\frac{1}{3}$ for mixed quantum states relative to pure quantum states that appears in the $O(\hbar^2)$ stress tensor (51).

IV. SMOOTHNESS PROPERTIES OF THE EFFECTIVE STRESS TENSOR

If the classical potential energy V has a discontinuity, then a δ function will appear on the right-hand sides of the QHD momentum and energy conservation equations (43) and (44). This δ function term is exactly canceled in Eq. (43) by a corresponding discontinuity in P_{ij}^Q and in Eq. (44) by corresponding discontinuities in P_{ij}^Q, W^Q, and $\mathbf{q}$, where the superscript Q denotes the quantum parts

$$P_{ij}^Q=-\frac{\hbar^2 n}{4mT}\frac{\partial^2\bar{V}}{\partial x_i\partial x_j}\ , \tag{59}$$

$$W^Q=\frac{\hbar^2 n}{8mT}\nabla^2\bar{V}\ . \tag{60}$$

We will first show that the second partial derivatives $\partial^2\bar{V}/\partial x_i\partial x_j$ of the quantum potential have the same degree of smoothness as the classical potential by showing that the Fourier transform $\bar{V}(\xi)$ of $\bar{V}(\mathbf{x})$ behaves like $\xi^{-2}V(\xi)$ as $|\xi|\rightarrow\infty$, where $V(\xi)$ is the Fourier transform of $V(\mathbf{x})$. Then the Fourier transform of $\partial^2\bar{V}/\partial x_i\partial x_j$ will behave like $\xi_i\xi_jV(\xi)/\xi^2$ and P_{ij}^Q and W^Q will have the same smoothness properties as V. Further, we will show that the leading singularity in $n\partial V/\partial x_j$ in Eq. (43) is exactly canceled by the leading singularity in $\partial P_{ij}^Q/\partial x_i$. In the derivation we will treat n and T as constants, since we are here concerned with the discontinuities in the highest spatial derivatives of V.

The quantum potential (47) is a convolution with Fourier transform

$$\bar{V}(\xi)=V(\xi)\int_0^\beta\frac{d\beta'}{\beta}\left[\frac{\beta'}{\beta}\right]^2\exp\left\{-\frac{(\beta-\beta')(\beta+\beta')\hbar^2}{8m\beta}\xi^2\right\}$$

$$=\frac{V(\xi)}{2\eta^2}\left[1-\frac{e^{-\eta^2}}{\eta}I(\eta)\right] \tag{61}$$

where $\eta=|\xi|\sqrt{\beta\hbar^2/8m}$ and $I(\eta)=\int_0^\eta ds\,e^{s^2}$. As

$|\xi|\to\infty$, $\exp\{-\eta^2\}I(\eta)\to 1/2\eta$ and

$$\bar{V}(\xi)\to\frac{4m}{\beta\hbar^2\xi^2}V(\xi)\ . \tag{62}$$

As $|\xi|\to\infty$, $\xi_i P^Q_{ij}(\xi)\to n\xi_j V(\xi)$. Now define the effective force F_j per unit volume in the momentum conservation equation (43) by moving the derivative of P^Q_{ij} to the right-hand side:

$$F_j(\mathbf{x})=\frac{\partial P^Q_{ij}}{\partial x_i}-n\frac{\partial V}{\partial x_j}\ . \tag{63}$$

The Fourier transform of $F_j(\mathbf{x})$ equals

$$F_j(\xi)=i\xi_i P^Q_{ij}(\xi)-i\xi_j nV(\xi)\to-\frac{4imnT}{\hbar^2}\frac{\xi_j V(\xi)}{\xi^2} \tag{64}$$

as $|\xi|\to\infty$. Thus the effective force F_j (63) is smoother by two degrees than the classical force $-\partial V/\partial x_j$; i.e., if V has a discontinuity, then F_j is continuous.

Some insight into the smoothing effects of the effective stress tensor may be gained by looking at a one-dimensional potential $V=V(x)$ and ignoring the spatial dependence of the density. We write the x component of the effective force as

$$\frac{F(x)}{n}=-\frac{dU}{dx}\ , \tag{65}$$

where the effective potential is

$$U\approx V+\frac{\hbar^2}{4mT}\frac{d^2\bar{V}}{dx^2}\ . \tag{66}$$

The term we have omitted in the approximation (66) is less singular than the terms we have kept. In QHD simulations of semiconductor derives [where we can solve for $n(x)$], the effective potential curves in Figs. 1–5 are modified by the addition of the smooth contribution

$$\frac{\hbar^2}{4m}\int^x\frac{dx}{nT}\frac{dn}{dx}\frac{d^2\bar{V}}{dx^2}\ . \tag{67}$$

The effective potential is plotted at $T=77$ and 300 K for electrons in GaAs in Figs. 3–5 for a potential step $V=V_0\theta(x)$, a potential barrier

$$V=V_0[\theta(x+a)-\theta(x-a)]\ , \tag{68}$$

and a double barrier

$$V=V_0[\theta(x+3a)-\theta(x+a)+\theta(x-a)-\theta(x-3a)]\ , \tag{69}$$

respectively, with $a=25$ Å. (The dependence of the effective electron mass m on T has been ignored in the figures.) The figures demonstrate that in the extended QHD model the discontinuous classical potential is replaced by a residual smoothed effective potential. For the single barrier (double barriers), the barrier height is re-

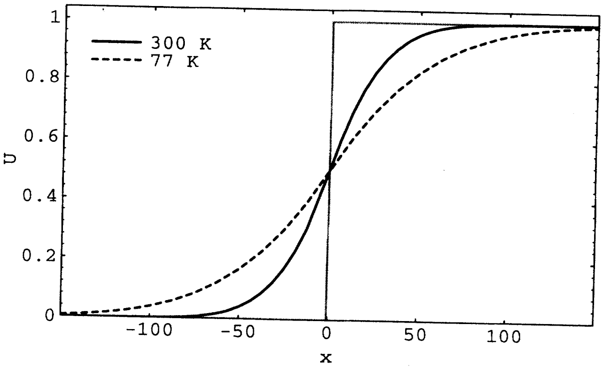

FIG. 3. Smooth effective potential U/V_0 for a potential step for electrons in GaAs at 300 and 77 K. x is in Å.

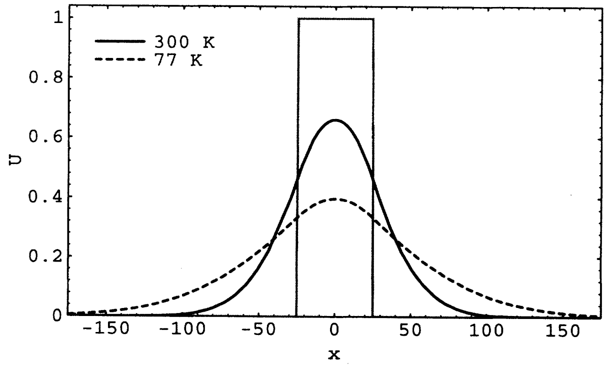

FIG. 4. Smooth effective potential U/V_0 for a potential barrier for electrons in GaAs at 300 and 77 K. x is in Å.

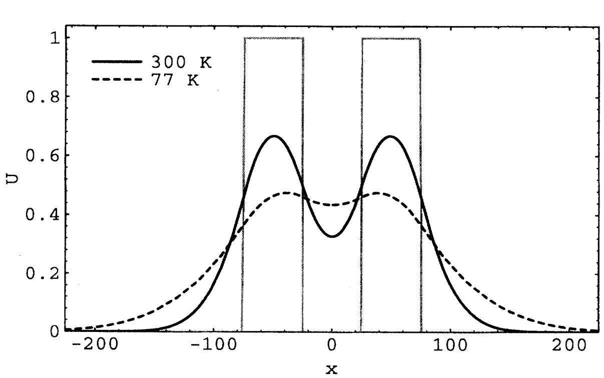

FIG. 5. Smooth effective potential U/V_0 for a double barrier for electrons in GaAs at 300 and 77 K. x is in Å.

duced by 35% (35%) at 300 K and 60% (50%) at 77 K. For the potential step, potential barrier, and double barrier, the quantum smoothing produces a repulsive force near the potential step or outer barrier edges that extends for roughly 75 Å at 300 K and 150 Å at 77 K. The reduced barrier height of U allows particles that classically would have been totally reflected at the potential discontinuity to penetrate the potential step or tunnel through the barriers. For the double barriers, note that the potential well in U is attractive yet much shallower than in V, and disappears as $T \to 0$.

To analyze what happens at a potential step $V(x,y,z)=V_0+\delta V\theta(x)$ when the dependence of the density on position is not ignored, we examine the jump conditions at $x=0$ for a stationary wave in which the state variables n, $\mathbf{u}$, and T are continuous and depend only on x. Integrating

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} dx \tag{70}$$

the QHD equations (42)–(44) across the wave, we obtain the jump relations

$$-\frac{\hbar^2}{4mT}\left[\frac{d^2\bar{V}}{dx^2}\right]=[V] , \tag{71}$$

$$\kappa\left[\frac{dT}{dx}\right]=-\frac{1}{2}nu\,[V] , \tag{72}$$

where the normal velocity $u=\hat{\mathbf{x}}\cdot\mathbf{u}$ and $[\chi]=\chi_+-\chi_-$ is the jump in χ across the wave. For concreteness, we have assumed that the heat flux $\mathbf{q}=-\kappa\nabla T$. Equation (71) says that the jump in the classical potential V is canceled by the jump in the quantum part of the stress tensor, as shown above, and Eq. (72) says that the jump in dT/dx is controlled by the jump in V.

We note here that since the leading discontinuity in the classical potential energy is canceled in the $O(\beta\nabla V)$ extended QHD equations, the $O((\beta\delta V)^2)$ corrections [see Eq. (86)] to the theory will be smooth, regardless of their magnitude.

V. CONCLUSION

The QHD equations derived here extend the range of validity of the original $O(\hbar^2)$ QHD theory since $P_{ij}=P_{ij}^{(2)}+O(\hbar^4)$. Further, the $O(\hbar^2)$ QHD equations were derived assuming that V is sufficiently smooth to have a Taylor series expansion, and that the expansion parameter $\hbar^2/8mTl^2 \ll 1$. The extended QHD theory only requires that $\beta\delta V \lesssim 20$, and is specifically designed to handle discontinuities in the classical potential. Discontinuities in ∇V on the right-hand sides of the QHD equations are exactly canceled by discontinuities in the first partial derivatives of P_{ij}, W, and $\kappa\delta T$ on the left-hand sides.

The jump relation (71) provides the mechanism by which particles can tunnel through a potential barrier in the QHD model. Classically, particles with energies below the barrier height are forbidden inside the barrier. In the QHD equations, the cancellations (71) and (72) make the barrier partially transparent to the particle flow, by eliminating the leading singularity in the classical potential and leaving a residual smooth effective potential (with a lower potential height) in the barrier region.

Finally we mention that the effective density matrix ρ given in Eq. (18) and its partition function $Z=\int d^3x\,\rho(\mathbf{x},\mathbf{x})$ may prove useful in their own rights for problems in quantum statistical mechanics.

Future investigations include mathematical results on the convergence of our iteration method for the solution to the Bloch equation and numerical simulations comparing solutions of the quantum Liouville equation and the extended QHD equations.

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APPENDIX A: RELATIONSHIP BETWEEN THE FEYNMAN-KLEINERT Z AND THE $O(\hbar^2)$ DISTRIBUTION FUNCTION

Feynman and Kleinert give the partition function $Z=\int dx\,\rho(x,x)$ as

$$Z=\int dx\left[\frac{m}{2\pi\beta\hbar^2}\right]^{1/2}\exp\left\{-\beta\left[\frac{1}{\beta}\ln\left[\frac{\sinh(\beta\Omega/2)}{\beta\Omega/2}\right]-\frac{ma^2\Omega^2}{2\hbar^2}+V_{a^2}(x)\right]\right\} , \tag{A1}$$

where the smeared potential is

$$V_{a^2}(x)=\int\frac{dy}{\sqrt{2\pi a^2}}\exp\left\{-\frac{(x-y)^2}{2a^2}\right\}V(y) \tag{A2}$$

and Ω^2 and a^2 are related through a variational principle by

$$\Omega^2(x)=\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2}V_{a^2}(x)=\frac{2\hbar^2}{m}\frac{\partial}{\partial a^2}V_{a^2}(x) , \tag{A3}$$

$$a^2=\frac{\hbar^2}{m\beta\Omega^2}\left[\frac{\beta\Omega}{2}\coth\left[\frac{\beta\Omega}{2}\right]-1\right] . \tag{A4}$$

In the high-temperature limit ($\beta \to 0$), $a^2 \approx \beta\hbar^2/12m$ and

$$Z \approx \int dx \left[\frac{m}{2\pi\beta\hbar^2} \right]^{1/2} \exp\left\{ -\beta V(x) - \frac{\hbar^2\beta^2}{24m} V''(x) \right\} , \tag{A5}$$

where we have used the fact that

$$V_{a^2}(x) = \sum_{n=0}^{\infty} \frac{a^{2n}}{(2n)!!} V^{(2n)}(x) . \tag{A6}$$

To compare the Feynman-Kleinert Z with the integral of the $O(\hbar^2)$ density matrix, we start with the $O(\hbar^2)$ thermal equilibrium solution [3] to the Wigner-Boltzmann equation:

$$f_W^{(2)}(\mathbf{x},\mathbf{p}) = \frac{e^{-\beta E}}{(2\pi\hbar)^3} \left[1 + \hbar^2 \left\{ -\frac{\beta^2}{8m} \frac{\partial^2 V}{\partial x_i^2} + \frac{\beta^2}{24m} \left[\frac{\partial V}{\partial x_i} \right]^2 + \frac{\beta^3 p_i p_j}{24m^2} \frac{\partial^2 V}{\partial x_i \partial x_j} \right\} \right] , \tag{A7}$$

where the classical energy $E = p^2/2m + V$. The integral of f_W with respect to $\mathbf{p}$ is the particle density

$$n(\mathbf{x},t) = \int d^3p\, f_W(\mathbf{x},\mathbf{p}) \approx \int d^3p\, f_W^{(2)}(\mathbf{x},\mathbf{p}) = \left[\frac{m}{2\pi\beta\hbar^2} \right]^{3/2} e^{-\beta V} \left[1 + \hbar^2 \left\{ -\frac{\beta^2}{12m} \frac{\partial^2 V}{\partial x_i^2} + \frac{\beta^3}{24m} \left[\frac{\partial V}{\partial x_i} \right]^2 \right\} \right] . \tag{A8}$$

Now we Fourier transform Eq. (A7) to obtain the density matrix:

$$\begin{aligned} \rho_W^{(2)}(\mathbf{x},\mathbf{y}) &= \int d^3p\, f_W^{(2)} \left[\frac{\mathbf{x}+\mathbf{y}}{2}, \mathbf{p} \right] e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})/\hbar} \\ &= \left[\frac{m}{2\pi\beta\hbar^2} \right]^{3/2} \exp\left\{ -\frac{m(\mathbf{x}-\mathbf{y})^2}{2\beta\hbar^2} - \beta V \right\} \\ &\quad \times \left[1 + \hbar^2 \left\{ -\frac{\beta^2}{12m} \frac{\partial^2 V}{\partial x_i^2} + \frac{\beta^3}{24m} \left[\frac{\partial V}{\partial x_i} \right]^2 - \frac{\beta}{24\hbar^2} (x_i - y_i)(x_j - y_j) \frac{\partial^2 V}{\partial x_i \partial x_j} \right\} \right] , \end{aligned} \tag{A9}$$

where V and its derivatives are evaluated at $(\mathbf{x}+\mathbf{y})/2$.

Note that $n(\mathbf{x},t) = \rho_W^{(2)}(\mathbf{x},\mathbf{x})$ agrees with Eq. (A8) and that

$$Z^{(2)} = \int d^3x\, \rho_W^{(2)}(\mathbf{x},\mathbf{x}) = \left[\frac{m}{2\pi\beta\hbar^2} \right]^{3/2} \int d^3x\, e^{-\beta V} \left[1 - \frac{\hbar^2\beta^2}{24m} \frac{\partial^2 V}{\partial x_i^2} \right] , \tag{A10}$$

which agrees with the three-dimensional generalization of the Feynman-Kleinert Z to $O(\hbar^2)$ as $\beta \to 0$.

APPENDIX B: AGREEMENT BETWEEN THE EFFECTIVE AND $O(\hbar^2)$ DENSITY MATRICES

The density matrix (18)

$$\rho(\beta,\mathbf{x},\mathbf{y}) \approx \rho_0(\beta,\mathbf{x},\mathbf{y})[1 - \beta\tilde{V}(\beta,\mathbf{x},\mathbf{y})] \tag{B1}$$

when expanded to $O(\hbar^2)$ using Eq. (25) reproduces the linear terms in V in the $O(\hbar^2)$ density matrix $\rho_W^{(2)}$ in Eq. (A9). The quadratic terms in V involving $(\partial V/\partial x_i)^2$, $V^2/2$, and $V\partial^2 V/\partial R_i \partial R_j$ come from the second iteration in the Neumann series solution to Eq. (13). To evaluate the effective density matrix to $O(\hbar^2)$, expand the potential terms in Eq. (25) about $\mathbf{R}$ to second order as

$$\frac{1}{2} \left[V \left[\mathbf{X}' + \mathbf{R} + \frac{\beta'}{2\beta} \mathbf{s} \right] + V \left[\mathbf{X}' + \mathbf{R} - \frac{\beta'}{2\beta} \mathbf{s} \right] \right] \approx V + X_i' \frac{\partial V}{\partial R_i} + \frac{1}{2} \left[X_i' X_j' + \frac{\beta'^2}{4\beta^2} s_i s_j \right] \frac{\partial^2 V}{\partial R_i \partial R_j} \tag{B2}$$

where it will be understood that without explicit arguments V and its derivatives are evaluated at $\mathbf{R}$. Plugging this expression back into Eq. (25) and integrating gives

$$\beta\tilde{V}(\beta,\mathbf{R},\mathbf{s}) \approx \beta V + \hbar^2 \left\{ \frac{\beta^2}{12m} \frac{\partial^2 V}{\partial R_i^2} + \frac{\beta}{24\hbar^2} s_i s_j \frac{\partial^2 V}{\partial R_i \partial R_j} \right\} . \tag{B3}$$

In counting powers of $\hbar$, $\mathbf{s}/\hbar$ is of order 1 in the density matrix, since under the Fourier transform it becomes $\mathbf{p}$ in the Wigner distribution function. Now using this approximation for the 6D quantum potential in Eq. (B1), we obtain the linear terms in V in the density matrix $\rho_W^{(2)}$.

To obtain the quadratic terms in V in $\rho_W^{(2)}$, we need to approximate the second iteration in the Neumann series solution to Eq. (13). The second iteration gives

$$\begin{aligned}\rho(\beta,\mathbf{R},\mathbf{s}) \approx \rho_2(\beta,\mathbf{R},\mathbf{s}) = {} & \rho_0(\beta,\mathbf{R},\mathbf{s}) - \beta\tilde{V}(\beta,\mathbf{R},\mathbf{s})\rho_0(\beta,\mathbf{R},\mathbf{s}) \\ & + \frac{\rho_0(\beta,\mathbf{R},\mathbf{s})}{2}\int_0^\beta d\beta' \int d^3R'\, d^3s' \left[\frac{m}{\pi(\beta-\beta')\hbar^2}\right]^3 \left[\frac{\beta}{\beta'}\right]^{3/2} \\ & \times \exp\left\{-\frac{2m}{(\beta-\beta')\hbar^2}R'^2 - \frac{m}{2\hbar^2}\frac{\beta}{\beta'(\beta-\beta')}s'^2\right\} \\ & \times \left[V\left[\mathbf{R}'+\frac{\mathbf{s}'}{2}+\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s}\right]\right. \\ & \left. + V\left[\mathbf{R}'-\frac{\mathbf{s}'}{2}+\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s}\right]\right] \left[\beta'\tilde{V}\left[\beta',\mathbf{R}'+\mathbf{R},\mathbf{s}'+\frac{\beta'}{\beta}\mathbf{s}\right]\right. . \end{aligned} \tag{B4}$$

Using Eq. (B3), we approximate $\beta'\tilde{V}$ as

$$\begin{aligned}\beta'\tilde{V}(\beta',\mathbf{R}'+\mathbf{R},\mathbf{s}'+\frac{\beta'}{\beta}\mathbf{s}) & \approx \beta' V(\mathbf{R}'+\mathbf{R}) + \hbar^2\left\{\frac{\beta'^2}{12m}\frac{\partial^2 V}{\partial R_i^2}(\mathbf{R}'+\mathbf{R}) + \frac{\beta'}{24\hbar^2}\left[s_i'+\frac{\beta'}{\beta}s_i\right]\left[s_j'+\frac{\beta'}{\beta}s_j\right]\frac{\partial^2 V}{\partial R_i\partial R_j}(\mathbf{R}'+\mathbf{R})\right\} \\ & \approx \beta' V + \beta' R_i'\frac{\partial V}{\partial R_i} + \frac{\beta'}{2}R_i'R_j'\frac{\partial^2 V}{\partial R_i\partial R_j} \\ & \quad + \hbar^2\left\{\frac{\beta'^2}{12m}\frac{\partial^2 V}{\partial R_i^2} + \frac{\beta'}{24\hbar^2}\left[s_i'+\frac{\beta'}{\beta}s_i\right]\left[s_j'+\frac{\beta'}{\beta}s_j\right]\frac{\partial^2 V}{\partial R_i\partial R_j}\right\} . \end{aligned} \tag{B5}$$

We also expand

$$\begin{aligned}\frac{1}{2}\left[V\left[\mathbf{R}'+\frac{\mathbf{s}'}{2}+\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s}\right]+V\left[\mathbf{R}'-\frac{\mathbf{s}'}{2}+\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s}\right]\right] & \\ \approx V + R_i'\frac{\partial V}{\partial R_i} + \frac{1}{2}\left[R_i'R_j' + \frac{s_i's_j'}{4} + \frac{\beta'^2}{4\beta^2}s_is_j + \frac{\beta'}{4\beta}(s_i's_j+s_is_j')\right]\frac{\partial^2 V}{\partial R_i\partial R_j} & \end{aligned} \tag{B6}$$

to second order. Plugging Eqs. (B5) and (B6) into Eq. (B4), we get

$$\begin{aligned}\rho(\beta,\mathbf{R},\mathbf{s}) \approx \rho_2(\beta,\mathbf{R},\mathbf{s}) \approx {} & \rho_0(\beta,\mathbf{R},\mathbf{s}) - \beta\tilde{V}(\beta,\mathbf{R},\mathbf{s})\rho_0(\beta,\mathbf{R},\mathbf{s}) \\ & + \rho_0(\beta,\mathbf{R},\mathbf{s})\left[\frac{\beta^2}{2}V^2 + \hbar^2\left\{\frac{\beta^3}{12m}V\frac{\partial^2 V}{\partial R_i^2} + \frac{\beta^2}{24\hbar^2}s_is_jV\frac{\partial^2 V}{\partial R_i\partial R_j} + \frac{\beta^3}{24m}\left[\frac{\partial V}{\partial R_i}\right]^2\right\}\right] . \end{aligned} \tag{B7}$$

The first three terms in brackets on the right-hand side of Eq. (B7) come from expanding

$$e^{-\beta V} \approx 1 - \beta V + \frac{\beta^2}{2}V^2 \tag{B8}$$

in Eq. (A9) for $\rho_W^{(2)}$, while the last term is the nonlinear term in V in $\rho_W^{(2)}/e^{-\beta V}$ missing in the Born approximation,

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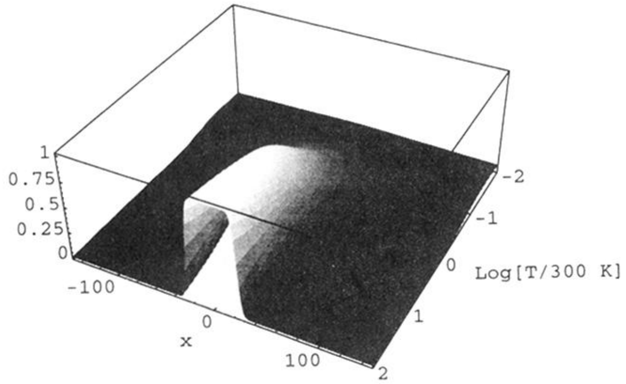

FIG. 1. Smooth effective potential for electrons in GaAs for a 50-Å-wide unit potential barrier as a function of x in Å and $\log_{10}\{T/[300\ (\mathrm{K})]\}$ for $3 \leq T \leq 30\,000$ K.