

Quantum hydrodynamic equations and quantum-hierarchy decoupling scheme

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(Received 6 May 2002; revised manuscript received 28 August 2002; published 16 December 2002)

There is a need to extract the relevant device physics from exact quantum transport formulations, and hence to reduce the complexity of quantum transport simulations for practical applications. We use a Hermite polynomial expansion to drastically reduce the number of degrees of freedom associated with the momentum variables. The result is a quantum hierarchy in real space. We also give a general procedure for the quantum-hierarchy decoupling scheme to derive the quantum hydrodynamic (QHD) and quantum drift-diffusion transport equations. We present some numerical results for the quantum hierarchy. A rigorous foundation of a decoupling procedure is given whereby the lower-order equations are renormalized in terms of a self-consistent effective potential, quantum diffusion coefficient, and moments, endowed with all the quantum corrections to order \hbar^2 . Our decoupling scheme is based on the general expression of $\text{Tr } \mathcal{H}^n$ to order \hbar^2 , valid at all temperatures without the need for expansion in terms of the small parameter and high temperature assumption. This is very important conceptually since existing QHD formulations, using expansion to order \hbar^2 , are based on a Boltzmann distribution with the restrictive assumption of a small parameter, which is not valid in abrupt heterojunction semiconductor devices. They also fail to account for important quantum nonlinearity in the form of nonequilibrium quantum corrections. These nonequilibrium quantum corrections are expected to play a major role in approximating the coherence manifested by the highly nonlinear current-voltage characteristics of resonant tunneling structures.

DOI: 10.1103/PhysRevE.66.066119

PACS number(s): 05.60.Gg, 85.35.-p, 85.30.De, 73.63.-b

I. INTRODUCTION

As is well known in the classical domain, the solution of distribution function transport equations entails large computing resources, and efforts to reduce the problem complexity are vigorously sought [1]. This task is even more demanding when solving quantum distribution function transport equations in terms of computational speed, memory, and numerical efficiency. Thus, there is a real need to reduce the problem size in numerically simulating quantum transport problems, both for fundamental study as well as for design optimization of optoelectronic and nanoelectronic devices. This work is motivated by the lack of an appropriately fast quantum transport solver for short channel and 12 Å gate oxide nano-complementary metal-oxide-silicon (CMOS) technology, nano-optoelectronic devices (multiband quantum transport dynamics), and heterostructure SiC-GaN high-power device technology, where quantum tunneling and coherence may play a significant role.

To significantly reduce the number of degrees of freedom associated with the momentum variables, we use the Hermite polynomial expansion of the quantum distribution function. The result is a “quantum hierarchy” in real space. We chose these basis functions since they possess desirable properties, namely, (a) they form “bounded” eigenfunctions of harmonic oscillators, and they are also eigenfunctions of the Fourier transform [2], (b) they are related to the Weyl transform and representation theory of the Heisenberg group in quantum mechanics, and as we shall see, (c) they provide a unified “spectral” resolution of the quantum and classical

distribution functions, thus illuminating the quantum corrections in more detail than previously. Their coefficients in the distribution function expansion provide the basis moments spanning the space of all physical moments.

In contrast with previous fragmented attempts to incorporate quantum effects in the potential or moments of the classical hydrodynamic transport equations [3], the method employed here is consistent and general without the need to expand in terms of a small parameter as was done by Wigner seven decades ago. The results are a straightforward consequence of the fundamental quantum distribution function transport equations. This lead to self-consistent quantum corrections to both the potential and moments of the quantum hydrodynamic (QHD) and quantum drift-diffusion (QDD) equations. In QDD, quantum diffusion, in the sense of stochastic quantum mechanics, is coherently taken into account together with the quantum potential. The procedure incorporates quantum coherence to $O(\hbar^2)$ which is often lacking in procedures based on *ad hoc* addition of a quantum correction to the potential in classical drift-diffusion equations.

The classical drift-diffusion and hydrodynamic transport equations *per se* do not have explicit quantum corrections. It is only when higher-order moment equations are considered that the quantum hydrodynamic equations differ from the classical hydrodynamic equations. This is also referred to here as the quantum hierarchy in real space. The practical need to consider only the first low-order Hermite coefficients or moments and low-order derivatives demands the renormalization of the potential and Hermite coefficients (or moments). It should be mentioned at the outset that any quantum-hierarchy decoupling scheme will have some restricted range of validity and predictive capability of the quantum mechanical effects. We will discuss a general decoupling procedure, which consistently renormalizes the po-

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tential and moments. This is done by deriving the general form of the stationary Wigner distribution function solution for any Hamiltonian system, expanded in powers of \hbar^2 .

The basic idea is that important quantum effects can be determined for the system under time-independent situations; transport simply adds asymmetry and additional nonequilibrium quantum corrections to the quantum distribution function. The whole of mesoscopic physics is in fact built on the assumption that quantum effects at equilibrium determine the allowed discrete quantum channels for transporting charge carriers [4]. This assumption is expected to be invalid for highly nonlinear and ultrafast quantum dynamics. The quantum-hierarchy decoupling technique proposed in this paper serves as a rigorous extension and generalization of the existing QHD formulations; see, for example, Ref. [5].

II. HERMITE POLYNOMIAL EXPANSION AND THE QUANTUM HIERARCHY IN REAL SPACE

The relevant Hermite polynomial is defined by the Rodrigues formula [6],

$$He_n(x) \equiv (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} = n! \sum_{m=0}^{[n/2]} (-1)^m \frac{(x)^{n-2m}}{m! 2^m (n-2m)!}. \quad (1)$$

The orthogonality of the relevant Hermite polynomials is expressed by $\int_{-\infty}^{\infty} e^{-x^2/2} He_n(x) He_m(x) dx = \sqrt{2\pi n!} \delta_{m,n}$. In what follows, let us take the dimensionless variable $x \Rightarrow \xi = p/\sqrt{m^*kT}$, and define the momentum basis states $\tilde{H}_m(p)$ as $He_n(x) \Rightarrow He_n(\xi) \equiv \tilde{H}_m(p)$. The orthogonality is expressed by $\int_{-\infty}^{\infty} e^{-p^2/2m^*kT} \tilde{H}_n(p) \tilde{H}_m(p) dp = \sqrt{2\pi m^*kT} n! \delta_{m,n}$. To illustrate the scheme for eliminating the momentum variables in the quantum transport equations, let us consider the single-band Wigner transport equation for a conventional resonant tunneling diode. We have the transport equation for the Wigner distribution function given by [7]

$$\begin{aligned} \frac{\partial}{\partial t} f_w(p, q, t) = & -\frac{p}{m^*} \nabla_q f_w(p, q, t) + \frac{2\pi}{h^4} \int dp' dv \left[V\left(q - \frac{v}{2}\right) \right. \\ & \left. - V\left(q + \frac{v}{2}\right) \right] \sin\left[\frac{(p-p')}{\hbar} v\right] f_w(p', q, t) \\ & + \left(\frac{\partial}{\partial t} f_w(p, q, t) \right)_{\text{collision}}. \end{aligned} \quad (2)$$

Since we are interested in quantum effects, we ignore for the moment any scattering contained in the collision term and consider only coupling to the Poisson equation for self-consistency of the potential. A differential form of Eq. (2) is the basis for gradient expansion theories. All these and the classical Boltzmann equations are included in the nonequilibrium Green's function equation by performing on it the "lattice" Weyl transformation appropriate for solid-state

problems [7,8]. A fully time-dependent one-dimensional (1D) numerical simulation of Eq. (2), coupled to the Poisson equation, was successfully initiated by Jensen and Buot [9]

For one-dimensional problem, we expand the 1D Wigner distribution function solution, based on dimensional grounds, as follows:

$$f_w^{1D}(p, q, t) = \sum_m \frac{2\pi m^*kT}{(2\pi\hbar)^2} f_m^w(q, t) e^{-p^2/2m^*kT} \tilde{H}_m(p). \quad (3)$$

The factor in front of the summation symbol allows the coefficients $f_m^w(q, t)$ to be dimensionless. The expansion is for each point q in real space so that the parameter T and mass m^* may be allowed to depend on (q, t) . In what follows, we will let $T(q, t)$ vary but treat m^* as a constant. $T(q, t)$ may be interpreted as the temperature of a shifted Maxwellian distribution; however, the expansion holds for a general Wigner distribution function.

The Hermite polynomial coefficients $f_m^w(q, t)$ are directly related to the average of the Hermite polynomials themselves, namely, $\langle \tilde{H}_n(p) \rangle \rho^w(q, t) = N_c n! f_n^w(q, t)$, where $\langle \tilde{H}_0(p) \rangle = 1$. N_c is given by $N_c = 2(2\pi m^*kT)^{3/2}/(2\pi\hbar)^3$. The moments for the particle density, momentum, and energy can be expanded in terms of Hermite coefficients, giving these coefficients a more elementary character as the basis moments, spanning the space of physical moments. The particle density distribution $\rho^w(q, t)$, particle-current density distribution $J(q, t)$, average kinetic energy density distribution $W(q, t)$, and energy density flux $\langle p^2 p/2m^* \rangle$, are given by $\rho^w(q, t) = N_c f_0^w(q, t)$, $J(q, t) = N_c \sqrt{kT/m^*} f_1^w(q, t)$, $W(q, t) = (N_c/2)kT\{f_0^w(q, t) + 2f_2^w(q, t)\}$, and $\langle p^2 p/2m^* \rangle = (N_c/2)\sqrt{kT/m^*} 3kT\{f_1^w(q, t) + 2f_3^w(q, t)\}$, respectively. Therefore, the m th moment of the Wigner distribution function with respect to the momentum variable is expanded in terms of the m th- and lower-order Hermite coefficients $f_n^w(q, t)$. This is not surprising since the Wigner distribution function can in principle be expanded in terms of either its moments or its correlation functions.

Substituting the expansion of $f_w(p, q, t)$ in terms of the Hermite polynomial in the Wigner distribution transport equation,

$$\begin{aligned} \sum_m \frac{\partial}{\partial t} \frac{2\pi m^*kT}{(2\pi\hbar)^2} f_m^w(q, t) e^{-p^2/2m^*kT} \tilde{H}_m(p) = & \sum_m \left\{ -\frac{p}{m^*} \nabla_q \frac{2\pi m^*kT}{(2\pi\hbar)^2} f_m^w(q, t) e^{-p^2/2m^*kT} \tilde{H}_m(p) \right. \\ & + \frac{2\pi}{h^4} \sum_m \frac{2\pi m^*kT}{(2\pi\hbar)^2} f_m^w(q, t) \int dp' dv \\ & \times \left. \left[\begin{array}{l} V\left(q - \frac{v}{2}\right) \\ -V\left(q + \frac{v}{2}\right) \end{array} \right] \sin\left[\frac{(p-p')}{\hbar} v\right] e^{-p'^2/2m^*kT} \tilde{H}_m(p') \right\}, \end{aligned} \quad (4)$$

yields the exact hierarchy of coupled equations for the Hermite coefficients, the quantum hierarchy,

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_j^w(q,t) = & -\nabla_q \left\{ (j+1) \sqrt{\frac{kT}{m^*}} N_c f_{j+1}^w(q,t) \right. \\ & \left. + \sqrt{\frac{kT}{m^*}} N_c f_{j-1}^w(q,t) \right\} \\ & + \frac{1}{\sqrt{2\pi m^* kT} j!} \sum_m \xi_{jm}(q) N_c f_m^w(q,t), \end{aligned} \quad (5)$$

where if j is even m is odd and vice versa. $\xi_{jm}(q)$ is given by the following exact expression:

$$\begin{aligned} \xi_{jm}(q) = & 8\pi^2 \sqrt{2\pi m^* kT} m! (i)^m \sum_{l=0}^{[m/2]} \left\{ He_j \left(-i \frac{\partial}{\partial y} \right) \right. \\ & \times \left[V \left(q + \frac{\hbar y}{2\sqrt{m^* kT}} \right) \right] e^{-y^2/2} \\ & \left. \times \frac{He_{m-2l}(y)}{l! 2^l (m-2l)!} \Big|_{y=0}^{y=\sqrt{m^* kT}/\hbar} \right\}, \end{aligned} \quad (6)$$

where in $He_j(-i\partial/\partial y)$ the variable argument is replaced by the differential operator. These are explicitly written here up to the fifth order equation, incorporating the \hbar^4 quantum correction, as

$$\begin{aligned} \frac{\partial}{\partial t} \begin{pmatrix} N_c f_0^w(q,t) \\ N_c f_1^w(q,t) \\ N_c f_2^w(q,t) \\ N_c f_3^w(q,t) \\ N_c f_4^w(q,t) \\ N_c f_5^w(q,t) \end{pmatrix} & = \begin{pmatrix} 0 & \mathcal{L}_{01} & 0 & 0 & 0 & 0 \\ \mathcal{L}_{10} & 0 & \mathcal{L}_{12} & 0 & 0 & 0 \\ 0 & \mathcal{L}_{21} & 0 & \mathcal{L}_{23} & 0 & 0 \\ \hbar^2 \mathcal{L}_{30}^Q & 0 & \mathcal{L}_{32} & 0 & \mathcal{L}_{34} & 0 \\ 0 & \hbar^2 \mathcal{L}_{41}^Q & 0 & \mathcal{L}_{43} & 0 & \mathcal{L}_{45} \\ \hbar^4 \mathcal{L}_{50}^Q & 0 & \hbar^2 \mathcal{L}_{52}^Q & 0 & \mathcal{L}_{54} & 0 \end{pmatrix} \\ & \times \begin{pmatrix} N_c f_0^w(q,t) \\ N_c f_1^w(q,t) \\ N_c f_2^w(q,t) \\ N_c f_3^w(q,t) \\ N_c f_4^w(q,t) \\ N_c f_5^w(q,t) \end{pmatrix}, \end{aligned} \quad (7)$$

where the matrix elements in powers of \hbar are quantum corrections which go to zero as $\hbar \Rightarrow 0$. The matrix elements are defined as follows:

$$\frac{\partial}{\partial t} N_c f_0^w(q,t) = -\nabla_q \sqrt{\frac{kT}{m^*}} N_c f_1^w(q,t), \quad (8)$$

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_1^w(q,t) = & -\nabla_q \left\{ 2 \sqrt{\frac{kT}{m^*}} N_c f_2^w(q,t) + \sqrt{\frac{kT}{m^*}} N_c f_0^w(q,t) \right\} \\ & + \left[\left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right] \right]_{\xi=q} \frac{1}{\sqrt{m^* kT}} N_c f_0^w(q,t), \end{aligned} \quad (9)$$

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_2^w(q,t) = & -\nabla_q \left\{ 3 \sqrt{\frac{kT}{m^*}} N_c f_3^w(q,t) + \sqrt{\frac{kT}{m^*}} N_c f_1^w(q,t) \right\} \\ & + \left[\left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right] \right]_{\xi=q} \frac{1}{\sqrt{m^* kT}} N_c f_1^w(q,t), \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_3^w(q,t) = & -\nabla_q \left\{ 4 \sqrt{\frac{kT}{m^*}} N_c f_4^w(q,t) + \sqrt{\frac{kT}{m^*}} N_c f_2^w(q,t) \right\} - \frac{\hbar^2}{24} \left[\left[\left(-\frac{\partial}{\partial \xi} \right)^3 V(\xi) \right] \right]_{\xi=q} \frac{1}{(\sqrt{m^* kT})^3} N_c f_0^w(q,t) \\ & + \left[\left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right] \right]_{y=0} \frac{1}{\sqrt{m^* kT}} N_c f_2^w(q,t), \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_4^w(q, t) = & -\nabla_q \left\{ 5 \sqrt{\frac{kT}{m^*}} N_c f_5^w(q, t) + \sqrt{\frac{kT}{m^*}} N_c f_3^w(q, t) \right\} - \frac{\hbar^2}{24} \left\{ \left(-\frac{\partial}{\partial \xi} \right)^3 \right\} [V(\xi)] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})^3} N_c f_1^w(q, t) \\ & + \left\{ \left(-\frac{\partial}{\partial \xi} \right) \right\} [V(\xi)] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})} N_c f_3^w(q, t), \end{aligned} \quad (12)$$

$$\begin{aligned} \frac{\partial}{\partial t} N_c f_5^w(q, t) = & -\nabla_q \left\{ 6 \sqrt{\frac{kT}{m^*}} N_c f_6^w(q, t) + \sqrt{\frac{kT}{m^*}} N_c f_4^w(q, t) \right\} + \frac{\hbar^4}{(16)(120)} \left[\left(-\frac{\partial}{\partial \xi} \right)^5 V(\xi) \right] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})^5} N_c f_0^w(q, t) \\ & - \frac{\hbar^2}{48} \left[\left(-\frac{\partial}{\partial \xi} \right)^3 V(\xi) \right] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})^3} N_c f_0^w(q, t) - \frac{\hbar^2}{12} \left[\left(-\frac{\partial}{\partial \xi} \right)^3 V(\xi) \right] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})^3} N_c f_2^w(q, t) \\ & + \left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right] \Big|_{\xi=q} \frac{1}{(\sqrt{m^* kT})} N_c f_4^w(q, t), \end{aligned} \quad (13)$$

where $V(\xi)$ is the self-consistent potential. The following equation corresponds to the equation for the second moment:

$$\begin{aligned} & \frac{\partial}{\partial t} kT [N_c f_0^w(q, t) + 2N_c f_2^w(q, t)] \\ & = -\nabla_q \left[N_c \sqrt{\frac{kT}{m^*}} 3kT f_1^w(q, t) + 2N_c \sqrt{\frac{kT}{m^*}} 3kT f_3^w(q, t) \right] \\ & + 2 \left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right] \Big|_{\xi=q} \sqrt{\frac{kT}{m^*}} N_c f_1^w(q, t). \end{aligned} \quad (14)$$

We have thus reduced the integro-differential Wigner transport equation to an exact differential equation involving only spatial variables. This is the domain of computational fluid dynamics (CFD), where several already well-established efficient computational techniques can be employed [10,11] (although the numerical handling of higher derivatives is mostly an uncharted domain even in turbulence CFD simulations).

We should point out that, to any order in \hbar^{2n} , the quantum-hierarchy equations can also be obtained using the differential form of Eq. (2) in phase space, namely,

$$\begin{aligned} \frac{\partial}{\partial t} f_w(p, q, t) = & -\frac{p}{m^*} \nabla_q f_w(p, q, t) \\ & + \sum_{n=0}^{\infty} \left(\frac{\hbar}{2} \right)^{2n} \frac{(-1)^n}{(2n+1)!} \frac{\partial^{2n+1}}{\partial q^{2n+1}} V(q) \\ & \times \frac{\partial^{2n+1}}{\partial p^{2n+1}} f_w(p, q, t), \end{aligned} \quad (15)$$

by using the identities $p\tilde{H}_m(p) = \sqrt{m^* kT} [\tilde{H}_{m+1}(p) + m\tilde{H}_{m-1}(p)]$, $(\partial/\partial p)\tilde{H}_m(p) = m\tilde{H}_{m-1}(p)/\sqrt{m^* kT}$, coupled with integration by parts. However, Eqs. (5) and (6) are exact, compact, and elegant.

The momentum variables were eliminated at the cost of introducing the indices for the Hermite polynomials, i.e., $f_j^w(q, t)$. The extension to 3D, although tedious, is straightforward by using the product of Hermite polynomials as basis functions, namely,

$$f_w(\vec{p}, \vec{q}, t) = \sum_{l,m,n} f_{l,m,n}^w(\vec{q}, t) e^{-\vec{p} \cdot \vec{p}/2m^* kT} \mathcal{G}_{l,m,n}(\vec{p}), \quad (16)$$

where the 3D basis function is $\mathcal{G}_{l,m,n}(\vec{p}) = \tilde{H}_l(p_x)\tilde{H}_m(p_y)\tilde{H}_n(p_z)$. Note that anisotropy in the effective mass m^* and temperature parameter T can be incorporated in the above 3D expansion if needed. The technique is similar to the method of moments for solving the classical Boltzmann equation.

We have given a mathematical recipe for the quantum distribution transport version, which is exact. The first approximation occurs when we impose closure on the hierarchy of ‘‘moment equations,’’ which is also a hierarchy of \hbar^2 quantum corrections, by using only a finite number of indices. An ideal way to close the hierarchy is to invoke a more rigorous procedure for decoupling the higher-order moments so as to bestow their quantum corrections, including nonlocality, on the lower-order moment equations under consideration. We will discuss this procedure in more detail later.

About 100 discrete points is a typical discretization of the momentum variables. If we truncate to two or five indices, this gives a factor of 50 or 20 reduction in the degrees of freedom associated with the momentum variables. The corresponding matrix or problem size is thus reduced by a factor of 2500 or 400. Further reduction in spatial variables by a factor of 10 is possible by using a multiquadric method [12], which will cause a total reduction in problem size by at least a factor of 40 000, i.e., four orders of magnitude. Thus for 3D quantum transport problems, there is a potential to reduce the size of the problems by several orders of magnitude, perhaps by a factor of more than 10^{12} . We hope to report our efforts on the multiquadric method, applied to Eq. (2) directly, in future communications.

The form of the classical Boltzmann equation under Hermite polynomial expansion without collision terms (ballistic case) and for the 1D case for comparison purposes can be readily obtained from the above results by simply taking the limit $\hbar \Rightarrow 0$. We see that the coupling of the coefficients in the Boltzmann equation is “nearest neighbor,” in the space of the Hermite coefficient discrete indices, compared to the quantum case, which gives a quantum correction to the lower-order coefficients via their coupling to the equations containing powers of \hbar^2 occurring at the third- and higher-order coefficients in the quantum hierarchy. Since these coefficients have direct relations to the moments, we see that quantum corrections emerge only in the equations for the third- and higher-order coefficients. This manner of incorporating quantum correction has the virtue of incorporating *quantum coherence under all nonequilibrium situations*. This means that the classical semiconductor hydrodynamic equations *per se* do not have any explicit quantum correction. This should be differentiated from quantum corrections of lower-order moments and potential, which naturally arise from the quantum correction of the transport equations of the coupled higher-order moments leading to the exact Wigner distribution function. Thus, a quantum-hierarchy decoupling scheme is needed to effectively deal only with low-order equations incorporating quantum coherence, at least to $O(\hbar^2)$.

It is worth mentioning that the difficulty of numerically handling higher derivatives for strongly varying potentials in order to capture quantum coherence and nonlocality may actually drive researchers to more serious research in finding alternative and efficient ways to numerically implement quantum distribution function transport equations. This is indeed foreseeable when addressing ultrafast and highly nonlinear quantum dynamics. We are also currently working on employing the multiquadric method to implement Eq. (2) numerically with a reduced number of degrees of freedom [12].

III. NUMERICAL RESULTS FOR THE QUANTUM HIERARCHY

We present some numerical results obtained from our numerical implementation of the coupled “bare” QHD or quantum-hierarchy equations, Eqs. (7), together with the appropriate boundary conditions. These equations are coupled to the Poisson equation for self-consistency in the potential. Our purpose here is simply to examine the complexity of the numerical simulation of the quantum correction to order \hbar^2 in Eqs. (8)–(13). For simplicity, we also treat T as uniform in the crystal lattice; thus N_c drops out from these equations. We will only present the results obtained by truncating Eqs. (7) to the third-order moment equation where the quantum correction first appear. We made calculations for transport across on $n^+ - i - n^+$ diode and single-barrier and double-barrier structures. We only calculate for the steady-state condition, whereby we can associate the third derivative of the strongly varying barrier potential with a derivative of smoother density functions, namely, $(-\partial/\partial q)^3 V(q) \approx kT(\partial/\partial q)^3 \ln\{f_0^w(q,t) + 2f_2^w(q,t)\}$, consistent with the

steady-state solution of Eq. (9), provided that $|f_2^w(q,t)| \ll f_0^w(q,t)$, consistent with our numerical result. Typically, for each bias the steady-state solution takes only few seconds to converge on a 1 GHz PC.

We have also avoided this association by using smooth barrier potentials and a smooth doping profile using the Gaussian approximation; we then take the potential derivative directly and also make use of the Poisson equation. The smoothness of our barrier potential can be adjusted through the use of the following barrier function:

$$V_B(q) = V_B^0 \left[1 - \left\{ \frac{(2 \arctan[(q-b)/a]/\pi + 1)}{2} + \frac{(-2 \arctan[(q+b)/a]/\pi + 1)}{2} \right\} \right], \quad (17)$$

where b determines the half width of the barrier, a determines the smoothness and steepness of the barrier edge, and V_B^0 is the barrier height or band-edge discontinuity. At steady state, $f_1^w(q,t)$, which determines the current density, becomes constant across the device.

Figure 1 shows the simulation results for the $n^+ - i - n^+$ diode, where we do not expect to find any quantum correction or tunneling correction to the current. For the smooth n^+ Gaussian doping we used a decay distance of 20 Å. Figure 2 shows the result for a single-barrier diode, constructed from the $n^+ - i - n^+$ diode of Fig. 1 by placing a barrier in the intrinsic i region (zero doping in the simulation). Equation (17) was used to construct the barrier potential with the following parameters: barrier halfwidth $b = 15$ Å, barrier decay length $a = 3$ Å, and barrier height $V_b^0 = 0.36$ V. In Fig. 3, the resonant tunneling diode (RTD) structure simulated has the same device parameters as the RTD used by Buot and Jensen [7] in their numerical simulation of the exact Wigner distribution transport equation, Eq. (2). Thus for the RTD simulated we employ abrupt doping through a Gaussian decay length of 10^{-3} Å, and an abrupt barrier potential with $a = 0.1$ Å in Eq. (17). We used a fully implicit time steepening scheme which simultaneously includes the Poisson equation together with the finite-volume discretization method. The even-indexed Hermite coefficients, e.g., f_0^w and f_2^w , are defined within the volume center, whereas the odd-indexed coefficients, e.g., f_1^w and f_3^w , are defined at the volume faces for numerical stability. Note that f_1^w and f_3^w are related to the particle current and heat flux. Steady-state solutions were obtained within a few seconds, since in the fully implicit method the time step can be made 100 ps to obtain the steady state.

For the double-barrier structure our calculations shows that quantum coherence or resonant tunneling is not captured to order \hbar^2 by the coupled “bare” QHD equations considered. In almost all diode structures considered, the currents are almost identical with those obtained by setting $\hbar \Rightarrow 0$. We conclude that to obtain coherence the equations for the higher-order moments, which give the nonlocality and off-diagonal long-range correlations in real space needed for tun-

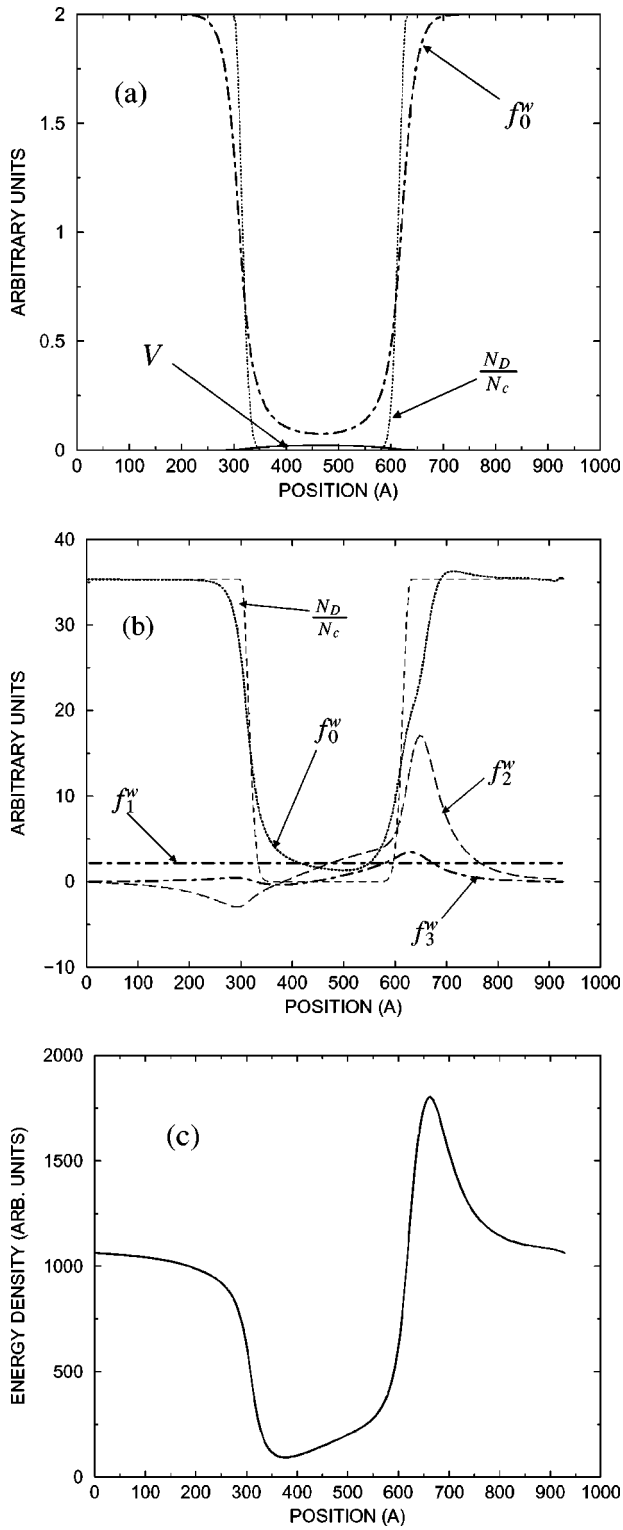


FIG. 1. (a) Simulated $n^+ - i - n^+$ diode at zero bias, showing the values of f_0^w , N_D/N_c , and potential V . N_D is the doping density and N_c is defined in the text; hence N_D/N_c is the “doping value” of f_0^w . (b) $n^+ - i - n^+$ diode at $V_{bias} = 0.04$ V showing the relative values of f_0^w , N_D/N_c , f_1^w , f_2^w , and f_3^w . The potential is not shown. The current value calculated corresponding to f_1^w is 2.62×10^5 A/cm². (c) Energy density distribution [proportional to $(f_0^w + 2f_2^w)$] at $V_{bias} = 0.04$ V.

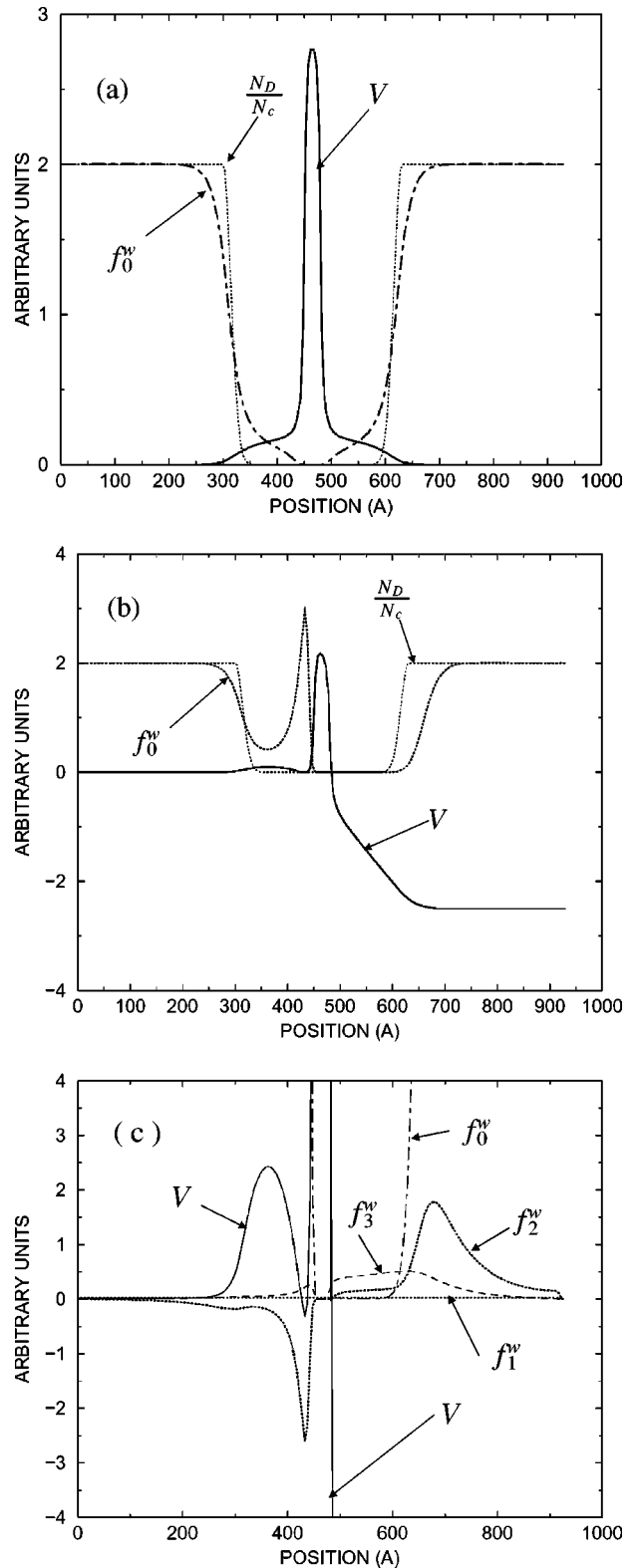


FIG. 2. (a) Single-barrier diode at $V_{bias} = 0.0$ V, showing N_D/N_c , f_0^w , and the potential. (b) $V_{bias} = 0.3$ V. (c) Magnified values of f_0^w , f_1^w , f_2^w , and f_3^w for $V_{bias} = 0.3$ V. The actual value of the current simulated from the constant value of f_1^w is 2600 A/cm². The solid line is the potential.

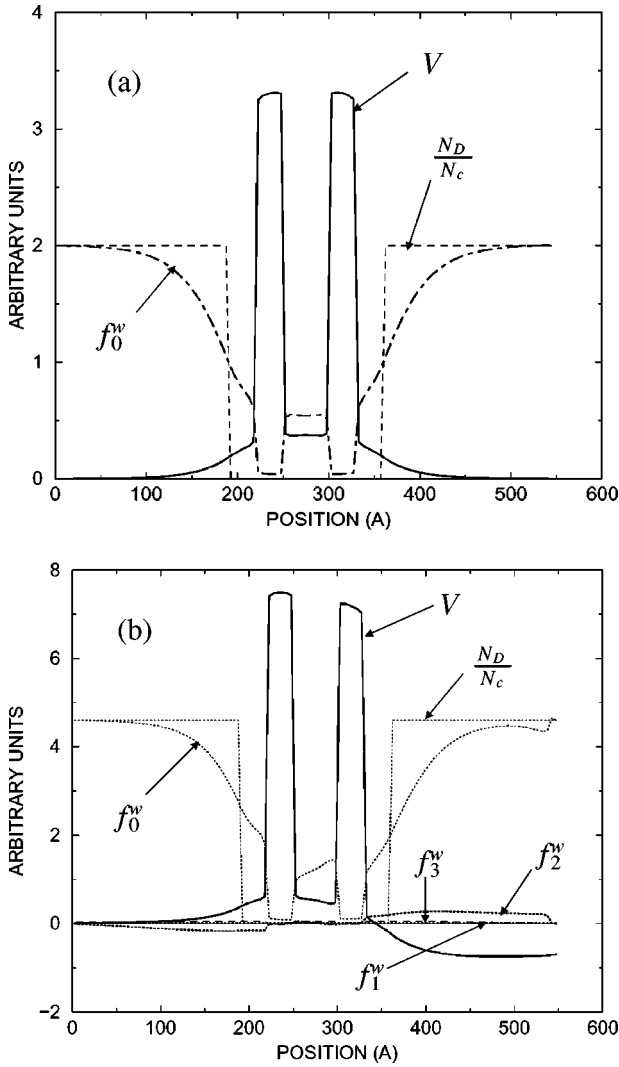


FIG. 3. (a) RTD diode at $V_{bias}=0.0$ V. (b) RTD diode at $V_{bias}=0.03$ V, showing the relative values of f_0^w , f_1^w , f_2^w , and f_3^w . The actual value of the current simulated from the constant value of f_1^w is 3.28×10^4 A/cm². The solid line is the double-barrier potential across the device.

neling and coherence, are very important. Clearly, the truncation to the third-order coefficients was not able to capture all the \hbar^2 corrections since the higher-order equations also contain \hbar^2 corrections. We note that, for the ballistic case considered, tunneling and coherence cannot be separated; the so-called sequential tunneling across double-barrier structures strictly occurs only if there is no inelastic scattering within the barriers but scattering occurs within the quantum well. In view of the difficulty in treating higher-order derivatives, it has become imperative that one accounts for the quantum corrections of the higher-order moments by renormalizing the lower-order moment equations through some sort of renormalization procedure. What we have also accomplished here is a demonstration of the usefulness of the Hermite polynomial expansion technique with the same complexity inherent in numerically simulating hydrodynamic transport equations.

IV. TRUNCATION-DECOUPLING SCHEME TO ORDER \hbar^2

Currently, *ad hoc* procedures for incorporating quantum effects fall into two general classes, namely, (a) construction of an effective potential [3], and (b) construction of the quantum hydrodynamic equations using an expansion of the Wigner distribution function in powers of \hbar^2 , based on the small-parameter perturbation theory described by Wigner seven decades ago [5]. Since the potential is modified directly in (a), clearly there will be differences in the calculated currents with and without quantum corrections. However, it is not clear that this type of renormalization captures the essential nonlocality for tunneling, and especially the coherence in double-barrier structures. Our preliminary investigation suggests that it does not capture coherence and resonant tunneling. In view of this, it seems uncertain whether the difference in the calculated current with and without quantum correction in (a) is due entirely to a quantum tunneling process. On the other hand, since it is the Wigner distribution function that is approximated in (b), it seems more likely that the essential nonlocality and off-diagonal long-range correlation in real space is captured in the resulting QHD equations. Although it is doubtful if the (b) approach can capture truly time-dependent or fast quantum transport processes, it should be useful enough to simulate semiconductor devices. In what follows, we will propose a self-consistent unification of the (a) and (b) approaches.

The approach used by Wigner [5] has in fact been generalized by one of the present authors (F.A.B.) three decades ago [13,14]. The derivation is not based on perturbation of a small parameter [5,15], but on the lattice Weyl-Wigner formalism for solid-state physics [13]. We summarize here the underlying philosophy of the lattice Weyl-Wigner derivation. The fundamental starting point is the formula derived by Buot [13] for the expansion in powers of \hbar^2 of $\text{Tr} A_{op}^n$, expressed in lattice phase-space representation, for any quantum operator A_{op} . In particular, for any solid-state Hamiltonian operator, $\text{Tr} \mathcal{H}^n$ is given by

$$\begin{aligned} \text{Tr} \mathcal{H}^n &= (N\hbar^3)^{-1} \text{Tr}_{band} \\ &\times \sum_{\vec{p}, \vec{q}} \cos \left[\frac{\hbar}{2} \sum_{\substack{j,k=1 \\ j < k}}^{n-1} \left(\frac{\partial^{(j)}}{\partial \vec{p}} \cdot \frac{\partial^{(k)}}{\partial \vec{q}} - \frac{\partial^{(j)}}{\partial \vec{q}} \cdot \frac{\partial^{(k)}}{\partial \vec{p}} \right) \right] \\ &\times \frac{1}{2} [H^{(1)}(\vec{p}, \vec{q}) H^{(2)}(\vec{p}, \vec{q}) \cdots H^{(n)}(\vec{p}, \vec{q}) \\ &+ H^{(n)}(\vec{p}, \vec{q}) H^{(n-1)}(\vec{p}, \vec{q}) \cdots H^{(1)}(\vec{p}, \vec{q})], \quad (18) \end{aligned}$$

where $H(\vec{p}, \vec{q})$ is the lattice Weyl transform of \mathcal{H} . $H(\vec{p}, \vec{q})$ is simply the classical expression of \mathcal{H} in most cases of single-band dynamics. However, for multiband cases each $H(\vec{p}, \vec{q})$ is a matrix in the band indices; they do not commute, and Tr_{band} must also be taken in Eq. (18). One may, however, decouple the bands, if possible, before applying the formula, as was done for a relativistic Dirac electron gas and the $\vec{k} \cdot \vec{p}$ model of bismuth-antimony alloys [13,14]. This formula has been shown to have a wide range of applications in solid-

state problems. This is connected with the fact that any function of \mathcal{H} , such as the free energy $F(\mathcal{K})$, where $\mathcal{K} = \mathcal{H} - \varepsilon_F$ and ε_F is the Fermi potential, can be expressed as a power series in \mathcal{K} through the use of the Laplace transform of $F(\mathcal{K})$ [16]:

$$\begin{aligned} F(\mathcal{K}) &= -kT \ln(1 + e^{-\mathcal{K}/kT}) \\ &= \int_{c-i\infty}^{c+i\infty} \phi(s) e^{s\mathcal{K}} ds, \\ e^{s\mathcal{K}} &= \sum_n \frac{s^n}{n!} \mathcal{K}^n. \end{aligned} \quad (19)$$

Hence the problem of taking the trace of $F(\mathcal{K})$ is reduced to the problem of taking $\text{Tr} \mathcal{K}^n$. Let \mathcal{N} be the total number of particles in the system. Then we have

$$\mathcal{N} = -\frac{\partial}{\partial \varepsilon_F} \text{Tr} F(\mathcal{K}) = (N\hbar^3)^{-1} \text{Tr}_{band} \sum_{\vec{p}, \vec{q}} f_w(\vec{p}, \vec{q}), \quad (20)$$

which defines the Wigner distribution function $f_w(\vec{p}, \vec{q})$. Thus an expansion of $\text{Tr} \mathcal{K}^n$ in powers of \hbar^2 will be reflected, through Eq. (19), in a similar expansion for the Wigner distribution function.

In Appendix A, we expand the cosine function in Eq. (18) to order \hbar^2 , and obtain the expression of the Wigner distribution to order \hbar^2 for any Hamiltonian, through Eq. (19). The result is

$$\begin{aligned} f_w(\vec{p}, \vec{q}) &= f(K(\vec{p}, \vec{q})) - \frac{\hbar^2}{8m^*} \nabla^2 V(q) f''(K(\vec{p}, \vec{q})) \\ &\quad - \frac{\hbar^2}{24m^*} |\nabla V(\vec{q})|^2 f'''(K(\vec{p}, \vec{q})) \\ &\quad - \frac{\hbar^2}{24m^{*2}} \vec{p} \cdot \nabla \nabla V(\vec{q}) \cdot \vec{p} f'''(K(\vec{p}, \vec{q})) \\ &\quad + \frac{\hbar^2}{8m^*} |\nabla V(\vec{q})|^2 \left(\frac{F(K)}{K} \right)'' \\ &\quad + \frac{\hbar^2}{8m^{*2}} \vec{p} \cdot \nabla \nabla V(\vec{q}) \cdot \vec{p} \left(\frac{F(K)}{K} \right)', \end{aligned} \quad (21)$$

where $f(K(\vec{p}, \vec{q}))$ is the Fermi-Dirac distribution function, and the differentiation is with respect to the scalar function $K(\vec{p}, \vec{q})$.

The task for the device quantum transport equation is to modify the equilibrium Fermi-Dirac distribution function appearing in Eq. (21) to a self-consistent nonequilibrium value. As a first approximation, we can assume a shifted Fermi-Dirac distribution function corresponding to a shift in the band-edge minimum in the parabolic band model, with the shifted momentum origin given in 1D by

$$\langle p \rangle_{FD}(q) = N_c \sqrt{m^* kT} f_1^{FD}(q) = u, \quad (22)$$

where $f_1^{FD}(q)$ is the first-order Hermite coefficient of the shifted Fermi-Dirac distribution. Although the treatment in 3D is straightforward, we will consider 1D here to simplify the discussion. We also expand the ‘‘1D’’ Fermi-Dirac distribution as

$$f_{FD}^{1D}(p, q, t) = \frac{2\pi m^* kT}{(2\pi\hbar)^2} \sum_m f_m^{FD}(q, t) e^{-p^2/2m^* kT} \tilde{H}_m(p). \quad (23)$$

With the essential quantum effects to order \hbar^2 already taken care of at equilibrium, we can solve for the nonequilibrium Fermi-Dirac distribution function by simply using its first few moments or coefficients of the Hermite polynomial expansion, i.e., we may employ the first two or three equations for the Hermite coefficients or of the moments. In capturing quantum effects, we can assume that the last two terms in Eq. (21) are negligible since these do not contribute at very low temperatures, and write $f_w(\vec{p}, \vec{q}, t)$ in one dimension as

$$\begin{aligned} f_w^{1D}(p, q, t) &= f^{1D}(K(p, q, t)) \\ &\quad - \frac{\hbar^2}{8m^*} \nabla^2 V(q) \frac{\partial^2}{\partial \varepsilon_F^2} f^{1D}(K(p, q, t)) \\ &\quad + \frac{\hbar^2}{24m^*} |\nabla V(q)|^2 \frac{\partial^3}{\partial \varepsilon_F^3} f^{1D}(K(p, q, t)) \\ &\quad + \frac{\hbar^2}{24m^{*2}} \nabla^2 V(q) \frac{\partial^3}{\partial \varepsilon_F^3} (p-u)^2 f^{1D}(K(p, q, t)), \end{aligned} \quad (24)$$

where $(p-u)^2$ in the last term is consistent with the fact that the shifted Fermi-Dirac distribution corresponds to a shift in the band-edge minimum in $K(\vec{p}, \vec{q}, t)$ by virtue of a drifting electron gas. We make use of the following relations to evaluate the Hermite polynomial expansion of the last term of Eq. (24):

$$\begin{aligned} \frac{p^2}{m^{*2}} \tilde{H}_m(p) &= \frac{kT}{m^*} [\tilde{H}_{m+2}(p) + (2m+1)\tilde{H}_m(p) \\ &\quad + m(m-1)\tilde{H}_{m-2}(p)], \\ -\frac{2pu}{m^{*2}} \tilde{H}_m(p) &= -\frac{2u}{m^*} \sqrt{\frac{kT}{m^*}} [\tilde{H}_{m+1}(p) + m\tilde{H}_{m-1}(p)], \end{aligned} \quad (25)$$

$$\frac{u^2}{m^{*2}} \tilde{H}_m(p) = \frac{u^2}{m^{*2}} \tilde{H}_m(p).$$

To simplify the equations that follows, let us denote the \hbar^2 factors as $A = (\hbar^2/m^*) \nabla^2 V(q) \partial^2 / \partial \varepsilon_F^2$, $B = (\hbar^2/m^*) |\nabla V(\vec{q})|^2 \partial^3 / \partial \varepsilon_F^3$, and $C = (\hbar^2/m^*) \nabla^2 V(\vec{q}) \partial^3 / \partial \varepsilon_F^3$. A

and B are dimensionless, whereas C has the dimension of inverse energy. The Wigner distribution function Hermite coefficients are related to the Fermi-Dirac distribution function Hermite coefficients, through Eq. (24), by the following:

$$\begin{aligned}
 f_m^w(q,t) &= \left[1 - \frac{A}{8} + \frac{B}{24} + (2m+1) \frac{CkT}{24} + \frac{C}{24m^*} u^2 \right] \\
 &\times f_m^{FD}(q,t) + \frac{CkT}{24} [f_{m-2}^{FD}(q,t) + (m+2)(m+1) \\
 &\times f_{m+2}^{FD}(q,t)] - \frac{C}{12} \sqrt{\frac{kT}{m^*}} u [f_{m-1}^{FD}(q,t) \\
 &+ (m+1)f_{m+1}^{FD}(q,t)]. \quad (26)
 \end{aligned}$$

Note that the Wigner distribution Hermite coefficients $f_m^w(q,t)$, are expanded as a linear combination of the Fermi-Dirac distribution Hermite coefficients, namely, $f_{m-2}^{FD}(q,t)$, $f_{m-1}^{FD}(q,t)$, $f_m^{FD}(q,t)$, $f_{m+1}^{FD}(q,t)$, and $f_{m+2}^{FD}(q,t)$. This is due to the presence of the last term in Eq. (24).

V. DERIVATION OF THE QUANTUM HYDRODYNAMIC TRANSPORT EQUATIONS

As we have indicated before, as a first simplification we can assume a momentum-shifted Fermi-Dirac distribution function. We will later consider nondegenerate semiconductors to make contact with existing formulations of QHD in the literature. We use the Hermite polynomial expansion of the Fermi-Dirac distribution $f^{1D}(\vec{p}, \vec{q}, t)$ of Eq. (23). We can readily identify the first three Hermite coefficients of the Fermi-Dirac distribution as follows: $N_c f_0^{FD}(q,t) = \rho(q,t)$, $N_c f_1^{FD}(q,t) = (u/\sqrt{m^*kT})\rho(q,t)$, $N_c f_2^{FD}(q,t) = (u^2/2m^*kT)\rho(q,t)$, and $N_c f_3^{FD}(q,t) = \{2/3! \sqrt{m^*kT} Q_{heat\ flux} / kT + 1/3! \rho(q,t) u^3(q,t) / (\sqrt{m^*kT})^3\}$. Expressing all coefficients in terms of the zero-order coefficient $f_0^{FD}(q,t)$, we have

$$\begin{aligned}
 f_1^{FD}(q,t) &= \frac{u}{\sqrt{m^*kT}} f_0^{FD}(q,t), \\
 f_2^{FD}(q,t) &= \frac{u^2}{2m^*kT} f_0^{FD}(q,t), \quad (27) \\
 f_3^{FD}(q,t) &= \left\{ \frac{2}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{kT \rho(q,t)} f_0^{FD}(q,t) \right. \\
 &\quad \left. + \frac{1}{3!} \frac{u^3(q,t)}{(\sqrt{m^*kT})^3} f_0^{FD}(q,t) \right\}.
 \end{aligned}$$

Therefore the Wigner distribution function Hermite coefficients can now be determined from Eq. (26). We have for $f_0^w(\vec{q}, t)$

$$f_0^w(\vec{q}, t) = \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] f_0^{FD}(\vec{q}, t), \quad (28)$$

and therefore in the nondegenerate limit we have

$$n(\vec{q}, t) = \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] \mathcal{A} e^{-(V/kT)}, \quad (29)$$

where $\mathcal{A} = 2[(2\pi m^*kT)^{3/2}/(2\pi\hbar)^3] e^{\varepsilon_F/kT}$. Note that the last term, notably absent in existing QHD formulations (see, e.g., Ref. [5]) is due to the presence of the ‘‘random’’ variable, i.e., the $(p-u)^2$ term in Eq. (24), which gives the ‘‘fluctuation’’ or thermal energy kT upon integration over the momentum variable. We also have to order \hbar^2 ,

$$\begin{aligned}
 \sqrt{\frac{kT}{m^*}} f_1^w(\vec{q}, t) &= \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] f_0^{FD}(q,t) \\
 &\times \left[\frac{u}{m^*} + \frac{C}{12} \frac{Q_{heat\ flux}}{\rho(q,t)} \right]. \quad (30)
 \end{aligned}$$

Thus the quantum-corrected velocity is defined by

$$v = \frac{u^w}{m^*} = \left(\frac{u}{m^*} + \frac{C}{12} \frac{Q_{heat\ flux}}{\rho(q,t)} \right). \quad (31)$$

This means that the quantum-corrected velocity is higher for non-Maxwellian classical distribution, i.e., in the presence of heat flux. The Wigner distribution particle current is thus given by

$$\begin{aligned}
 J(q,t) &= N_c \sqrt{\frac{kT}{m^*}} f_1^w(\vec{q}, t) \\
 &= n(q,t) \frac{u^w}{m^*}. \quad (32)
 \end{aligned}$$

To order \hbar^2 , we can write $n(q,t)(C/12)Q_{heat\ flux}/\rho(q,t) \approx (C/12)Q_{heat\ flux}$. Thus, the continuity equation is

$$\begin{aligned}
 \frac{\partial}{\partial t} n(q,t) &= -\nabla \frac{n(q,t)u}{m^*} \\
 &\quad - \frac{\hbar^2}{12m^*} \nabla \left(\nabla^2 V(\vec{q}) \frac{1}{(kT)^3} Q_{heat\ flux} \right). \quad (33)
 \end{aligned}$$

This differs from that given in existing QHD formulations by the absence of the last term of Eq. (33) in Ref. [5]. Equation (33) amounts to the replacement of u in Ref. [5] by u^w , the quantum-corrected momentum, thereby giving the usual continuity equation

$$\frac{\partial}{\partial t} n(q,t) = -\nabla \frac{n(q,t)u^w}{m^*} = -\nabla n(q,t)v. \quad (34)$$

For the second-order coefficient, we have

$$\begin{aligned} f_2^w(q,t) &= \left[1 - \frac{A}{8} + \frac{B}{24} + 5\frac{CkT}{24} + \frac{C}{24m^*}u^2 \right] \\ &\times \frac{u^2}{2m^*kT} f_0^{FD}(q,t) + \left[\frac{CkT}{48} + \frac{3C}{24} \frac{Q_{heat\ flux}}{\rho(q,t)(kT)} u \right. \\ &\left. - \frac{C}{24m^*}u^2 \right] f_0^{FD}(\vec{q},t), \end{aligned} \quad (35)$$

where we made use of the expression for $f_4^{FD}(q,t)$ in terms of the moments and $f_0^{FD}(\vec{q},t)$ derived in Appendix C. Taking the velocity moment of the Wigner distribution function equation gives the current equation

$$\begin{aligned} \frac{\partial}{\partial t} \sqrt{\frac{kT}{m^*}} N_c f_1^w(q,t) \\ = -\nabla_q \left\{ 2\frac{kT}{m^*} N_c f_2^w(q,t) + \frac{kT}{m^*} N_c f_0^w(q,t) \right\} \\ + \frac{1}{m^*} \left\{ \left(-\frac{\partial}{\partial q} \right) V(q) \right\} N_c f_0^w(q,t). \end{aligned} \quad (36)$$

Note that, from Eq. (9), this looks like multiplying both sides of Eq. (9) by $\sqrt{kT/m^*}$, but with a very important difference, namely, the factor $\sqrt{kT/m^*}$ is inside the differentiation operator since it depends on (q,t) . Upon substituting the relevant expressions given above, we end up with the quantum-corrected current equation to order \hbar^2 as

$$\mathcal{D}_{eff}(q) = \left[kT + m^*v^2 + \frac{\hbar^2 n(\vec{q},t)}{24m^*kT} \nabla^2 V(q) + \frac{\hbar^2}{12(kT)^3} \nabla^2 V(q) \frac{Q_{heat\ flux}}{\rho(q,t)} v + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q)v^2 + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q)v^4 \right], \quad (40)$$

$$\begin{aligned} \mathcal{V}_{eff}(q) &= \left[V(q) + kT + m^*v^2 + \frac{\hbar^2 n(\vec{q},t)}{24m^*kT} \nabla^2 V(q) + \frac{\hbar^2}{12(kT)^3} \nabla^2 V(\vec{q}) \frac{Q_{heat\ flux}}{\rho(q,t)} v + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q)v^2 \right. \\ &\left. + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q)v^4 \right]. \end{aligned} \quad (41)$$

The evolution equation for the energy is obtained from a combination of the equation for $f_0^w(q,t) + 2f_2^w(q,t)$. First, let us examine the expression for the total energy, namely,

$$\begin{aligned} \frac{\partial}{\partial t} [m^*n(q,t)v] + \nabla_q [m^*n(q,t)v^2 - \hbar^2 P_p] \\ = \left(-\frac{\partial}{\partial q} V(q) \right) n(q,t) - \nabla_q [n(q,t)kT] \\ + \left(\frac{\partial}{\partial t} m^*n(q,t)v \right)_c, \end{aligned} \quad (37)$$

where

$$\begin{aligned} P_p &= -\frac{n(q,t)}{24m^*kT} \nabla^2 V(q) \\ &- \left[\frac{1}{12(kT)^3} \nabla^2 V(q) \frac{Q_{heat\ flux}}{\rho(q,t)} v \right. \\ &\left. + \frac{1}{12(kT)^2} \nabla^2 V(q)v^2 + \frac{m^*}{24(kT)^3} \nabla^2 V(q)v^4 \right] \\ &\times n(q,t). \end{aligned} \quad (38)$$

We should point out that Gardner [5] missed out the \hbar^2 terms involving the quantum-corrected velocity v in the left-hand side of the current equation given above. These are inherently dynamical and nonequilibrium quantum corrections. We believe these represent an important quantum nonlinearity needed to preserve some amount of coherence in $O(\hbar^2)$. Clearly, to obtain the highly nonlinear current-voltage relationship in resonant tunneling structures one needs highly nonlinear terms as given in Eq. (37). These quantum corrections can also be interpreted as quantum corrections to the ‘‘ballistic’’ diffusion coefficient and the potential as

$$\begin{aligned} \frac{\partial}{\partial t} m^*n(q,t)v &= \left\{ \left(-\frac{\partial}{\partial q} \right) \mathcal{V}_{eff} \right\} n(q,t) - \mathcal{D}_{eff} \nabla_q n(q,t) \\ &+ \left(\frac{\partial}{\partial t} m^*n(q,t)v \right)_c, \end{aligned} \quad (39)$$

where

$$\begin{aligned}
 W(q,t) &= \frac{N_c}{2} kT [f_0^w(q,t) + 2f_2^w(q,t)] \\
 &= \frac{N_c}{2} \left(\left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] f_0^{FD}(q,t) kT + \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] \frac{u^2}{m^*} f_0^{FD}(q,t) \right. \\
 &\quad \left. + \left[\frac{2C(kT)^2}{48} + \frac{6C}{24} \frac{Q_{heat\ flux}}{\rho(q,t)} u + \frac{2CkT}{24m^*} u^2 + \frac{C}{24m^*} \frac{u^4}{m^*} \right] f_0^{FD}(q,t) \right). \quad (42)
 \end{aligned}$$

To order \hbar^2 , we have

$$(u^w)^2 = u^2 + \frac{2Cm^*}{12} \frac{Q_{heat\ flux}}{\rho(q,t)} u. \quad (43)$$

Then we end up with

$$W(q,t) = \left(\frac{kT}{2} + \frac{u^{w2}}{2m^*} + \frac{\hbar^2}{48m^*kT} \nabla^2 V(q) \left[1 + \frac{2Q_{heat\ flux}}{(kT)^2 \rho(q,t)} u^w + \frac{u^{w2}}{m^*kT} + \frac{u^{w4}}{m^{*2}(kT)^2} \right] \right) n(q,t). \quad (44)$$

Note that the leading quantum correction to the total energy is similar to that given by Wigner several decades ago; it differs by a factor of $\frac{1}{2}$ since we have also included the contribution of nonequilibrium-induced higher-order moments, specifically the contribution of f_4^{FD} (see Appendix C), which is made available by using the spectral resolution using the Hermite polynomials. Moreover, even the average momentum u^w is also a quantum-corrected momentum by virtue of the dynamical corrections. All the rest are dynamical and nonequilibrium quantum corrections not present in Ref. [5].

From Eq. (14), we have the following expression:

$$\begin{aligned}
 \frac{\partial}{\partial t} W(q,t) &= -\nabla_q \left\{ 3 \sqrt{\frac{kT}{m^*}} kT N_c f_3^w(q,t) \right. \\
 &\quad \left. + \frac{3}{2} \sqrt{\frac{kT}{m^*}} kT N_c f_1^w(q,t) \right\} \\
 &\quad + \left[\left(-\frac{\partial}{\partial \xi} \right) V(\xi) \right]_{\xi=q} \frac{1}{\sqrt{m^*kT}} kT N_c f_1^w(q,t). \quad (45)
 \end{aligned}$$

Upon substituting the Wigner Hermite coefficients in terms of the classical moments (Appendixes B–D), we obtain

$$\begin{aligned}
 \frac{\partial}{\partial t} W(q,t) &= -\nabla_q \left\{ W(q,t)v + kTn(q,t)v - \frac{\hbar^2}{m^*} \nabla^2 V(q) \left[\frac{n(q,t)}{16kT} v + \frac{23}{24(kT)^3} Q_{heat\ flux} \frac{m^* v^2}{2} \right. \right. \\
 &\quad \left. \left. + \frac{7n(\vec{q},t)}{24(kT)^2} \frac{m^* v^3}{2} + \frac{3n(\vec{q},t)}{24(kT)^3} \frac{m^* v^5}{2} \right] + \frac{\hbar^2}{m^*} \nabla^2 V(q) \left[\frac{1}{48kT} \sqrt{\frac{kT}{m^*}} n(q,t) - \frac{1}{4(kT)^2} Q_{heat\ flux} \right] \right. \\
 &\quad \left. + \left[1 + \frac{\hbar^2}{24m^*(kT)^3} |\nabla V(q)|^2 \right] Q_{heat\ flux} \right\} + \left(-\frac{\partial}{\partial q} \right) V(q)n(q,t)v, \quad (46)
 \end{aligned}$$

which can be written as

$$\begin{aligned}
 \frac{\partial}{\partial t} W(q,t) + \nabla_q [W(q,t)v(q,t) - \hbar^2 P_w(q,t)v(q,t)] &= \left(-\frac{\partial}{\partial q} V(q) \right) n(q,t)v(q,t) - \nabla_q kTn(q,t)v(q,t) \\
 &\quad - \nabla_q Q_{heat\ flux}(q,t) + \left(\frac{\partial}{\partial t} W(q,t) \right)_c, \quad (47)
 \end{aligned}$$

where

$$P_W = \frac{n(q,t)}{16m^*kT} \nabla^2 V(q) + \left\{ \frac{1}{m^*} \nabla^2 V(\vec{q}) \left[+ \frac{23}{24(kT)^3} Q_{heat\ flux} \frac{m^*v}{2} + \frac{7n(\vec{q},t)}{24(kT)^2} \frac{m^*v^2}{2} + \frac{3n(\vec{q},t)}{24(kT)^3} \frac{m^*v^4}{2} \right] \right. \\ \left. - \frac{1}{m^*} \nabla^2 V(\vec{q}) \left[\frac{1}{48kT} \frac{\sqrt{kT/m^*}}{v} n(q,t) - \frac{1}{4(kT)^2} \frac{1}{v} Q_{heat\ flux} \right] - \frac{1}{24m^*(kT)^3} |\nabla V(\vec{q})|^2 \frac{1}{v} Q_{heat\ flux} \right\}. \quad (48)$$

We may also cast the energy conservation equation in terms of heat generation and heat loss on the right-hand side as follows:

$$\frac{\partial}{\partial t} W(q,t) = \left(- \frac{\partial}{\partial q} V_{eff}^W(q) \right) n(q,t)v(q,t) - D_{eff}^W \nabla_q n(q,t)v(q,t) - \nabla_q Q_{heat\ flux}(q,t) + \left(\frac{\partial}{\partial t} W(q,t) \right)_c, \quad (49)$$

where

$$V_{eff}^W(q) = V(q) + \frac{3kT}{2} + \frac{m^*v^2}{2} + \frac{\hbar^2}{12m^*kT} \nabla^2 V(q) + \frac{\hbar^2}{48m^*kT} \nabla^2 V(q) \left[\frac{m^*v^2}{kT} + \frac{m^*v^4}{(kT)^2} \right] \\ - \frac{\hbar^2}{m^*} \nabla^2 V(q) \left[\frac{7}{24(kT)^2} \frac{m^*v^3}{2} + \frac{3}{24(kT)^3} \frac{m^*v^5}{2} \right] + \frac{\hbar^2}{48m^*kT} \nabla^2 V(q) \frac{\sqrt{kT}}{v} + \frac{\hbar^2}{24m^*(kT)^3} |\nabla V(q)|^2 \frac{Q_{heat\ flux}}{nv} \\ - \frac{\hbar^2}{4m^*(kT)^2} \nabla^2 V(q) \frac{Q_{heat\ flux}}{nv} + \frac{\hbar^2}{48m^*(kT)^3} \nabla^2 V(q) m^*v \frac{2Q_{heat\ flux}}{nv} - \frac{23\hbar^2}{24m^*(kT)^3} \nabla^2 V(q) \frac{m^*v^2}{2} \frac{Q_{heat\ flux}}{nv} \quad (50)$$

and

$$D_{eff}^W = V_{eff}^W(q) - V(q). \quad (51)$$

For the heat flux, we substitute $Q_{heat\ flux} = -\kappa \nabla T$ in all the formulas above, where κ is the thermal conductivity. The validity of this heat-flux formula and the Wiedemann-Franz law in the quantum domain has recently been discussed in Ref. [17]. We believe that physically meaningful quantum corrections should be in the form of the quantum corrections to the effective potential $V_{eff}^W(q)$, in the sense of Bohm Hamilton-Jacobi-particle dynamics, and to D_{eff}^W for the quantum diffusion, in the sense of the stochastic formulation of quantum mechanics [18], as given above.

Summarizing, we have the QHD equations Eq. (34), Eqs. (37),(38), and Eqs. (47),(48) cast in the form given by Gardner [5] for comparison. These are the forms of the QHD equations given in the literature [5]. The leading correction of the energy conservation equation differs from that given by Gardner [5] in sign and is $\frac{3}{4}$ in magnitude. However, the corresponding leading term in the effective potential in Eq. (50) is the same as the one used in [3]. The dynamical terms within the curly brackets in Eq. (48) were entirely missed in [5]. The leading-term discrepancy is attributed to the contribution of higher-order moments or Hermite coefficients which are not accounted for in the strictly equilibrium Wigner-function-based quantum corrections that characterize the procedure in [5]. Just as we did for the current equation, these extra quantum corrections can also be similarly interpreted as the quantum correction to the work done by the

electron pressure and to the effective potential. From the nonequilibrium quantum-mechanical point of view, Eqs. (34), (39), and (49) are the physically more meaningful version of the QHD equations.

VI. THE QUANTUM DRIFT-DIFFUSION EQUATIONS

In cases where the temperature is uniform and in equilibrium with the crystal lattice, we only need the continuity or particle conservation equation and the current equation. These are the workhorse equations of semiconductor device physics. Even if the temperature varies, it maybe desirable to truncate the hierarchy to these two equations only if the temperature variation is given, otherwise one has to solve the QHD equations to obtain the variation of temperature $T(q,t)$. We will treat the two cases, uniform T and given variable $T(q)$, in what follows. The quantum drift-diffusion equations follow from these two equations. Careful attention must be paid to the relaxation times in deriving the semiconductor QDD equations from the continuity equation and current equation given above. We note that their relaxation times have a very large discrepancy if one considers the relaxation time τ_d for the particle density n to be infinite, i.e.,

$$\tau_d \gg \tau_m, \quad (52)$$

where the particle-density relaxation time $\tau_d \Rightarrow \infty$ and τ_m is the finite (say 10^{-14} s) momentum relaxation time. Rewriting the particle conservation equation as

$$\frac{\partial}{\partial t} n = -\nabla n v - \frac{n - n_0}{\tau_d}, \quad (53)$$

and setting the collision term $[(\partial/\partial t)m^*nv]_c = -m^*nv/\tau_m$ for the current equation, we have

$$\begin{aligned} & \frac{\partial}{\partial t} (m^*nv) + \nabla_q [m^*nv^2 - \hbar^2 P_p] \\ &= \left(-\frac{\partial}{\partial q} V(q) \right) n - \nabla_q (nkT) - \frac{m^*nv}{\tau_m}. \end{aligned} \quad (54)$$

Because the current nv relaxes infinitely fast compared to n , τ_m introduces an elementary time scale to the problem. It is a very good approximation to assume that the current has already relaxed while following the current continuity equation, and hence we can set $(\partial/\partial t)(m^*nv) = 0$. This approximation is also good even if there are generation and recombination terms in the particle conservation equation, as long as the generation and recombination rates are much smaller than the momentum relaxation rate. We have

$$\begin{aligned} nv &= \frac{\tau_m}{m^*} \left(-\frac{\partial}{\partial q} V(q) \right) n - \nabla_q \frac{\tau_m}{m^*} (nkT) \\ &\quad - \nabla_q \frac{\tau_m}{m^*} [m^*nv^2 - \hbar^2 P_p]. \end{aligned} \quad (55)$$

First we treat the uniform T case. Then we obtain

$$J = e\mu\mathcal{E}n + eD\nabla_q(n) + \mu\nabla_q[m^*nv^2 - \hbar^2 P_p], \quad (56)$$

where μ is the electron mobility, D is the electron diffusion constant, and $J = -env$ is opposite to the direction of the electron velocity v . We immediately get the first version of the QDD equations as

$$\frac{\partial}{\partial t} n = -\nabla n v, \quad (57)$$

$$J = e\mu\mathcal{E}n + eD\nabla_q(n) + \mu\nabla_q[m^*nv^2 - \hbar^2 P_p], \quad (58)$$

where

$$\begin{aligned} P_p &= -\frac{n}{24m^*kT} \nabla^2 V(\vec{q}) - \left[\frac{1}{12(kT)^2} \nabla^2 V(\vec{q}) v^2 \right. \\ &\quad \left. + \frac{m^*}{24(kT)^3} \nabla^2 V(\vec{q}) v^4 \right] n. \end{aligned} \quad (59)$$

We may also take the physically meaningful point of view that the quantum corrections contained in P_p are absorbed as quantum corrections to the potential and diffusion constant. Then we have the second version of the QDD equations, which reads

$$\frac{\partial}{\partial t} n = -\nabla n v, \quad (60)$$

$$J = e\mu\mathcal{E}_{eff}n + eD_{eff}\nabla_q(n) + \mu\nabla_q(m^*nv^2), \quad (61)$$

where

$$\begin{aligned} e\mathcal{E}_{eff} &= \nabla \left\{ V(q) + \frac{\hbar^2}{24m^*kT} \nabla^2 V(q) + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q) v^2 \right. \\ &\quad \left. + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q) v^4 \right\}, \end{aligned} \quad (62)$$

$$\begin{aligned} D_{eff} &= \frac{\mu}{e} \left\{ kT + \frac{\hbar^2}{24m^*kT} \nabla^2 V(q) + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q) v^2 \right. \\ &\quad \left. + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q) v^4 \right\}. \end{aligned} \quad (63)$$

Note that the presence of the last term in the current equation comes from the contribution of the second-order or kinetic energy moment in the hierarchy, namely, $f_2^w(\vec{q}, t)$ or $\langle \tilde{H}_2(p) \rangle \rho^w(q, t)$. This is not a quantum correction but a higher-order moment correction and is partly responsible for the classical velocity-overshoot mechanism in GaAs devices. We can also absorb this term in the effective potential and diffusion coefficient to obtain the third version of the QDD equations as

$$\frac{\partial}{\partial t} n = -\nabla n v, \quad (64)$$

$$J = e\mu\tilde{\mathcal{E}}_{eff}n + e\tilde{D}_{eff}\nabla_q(n), \quad (65)$$

where

$$\begin{aligned} e\tilde{\mathcal{E}}_{eff} &= \nabla \left\{ V(q) + m^*v^2 + \frac{\hbar^2}{24m^*kT} \nabla^2 V(q) \right. \\ &\quad \left. + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q) v^2 + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q) v^4 \right\}, \end{aligned} \quad (66)$$

$$\begin{aligned} \tilde{D}_{eff} &= \frac{\mu}{e} \left\{ kT + m^*v^2 + \frac{\hbar^2}{24m^*kT} \nabla^2 V(q) \right. \\ &\quad \left. + \frac{\hbar^2}{12(kT)^2} \nabla^2 V(q) v^2 + \frac{\hbar^2 m^*}{24(kT)^3} \nabla^2 V(q) v^4 \right\}. \end{aligned} \quad (67)$$

Note the coherent quantum corrections to $\tilde{\mathcal{E}}_{eff}$ and \tilde{D}_{eff} for the QDD equations. We can express the derivatives of the potential $V(\vec{q})$ in terms of derivatives of $\ln n$. In Eq. (29), we take the logarithm of both sides of the equation to obtain

$$-V = kT \ln n - kT \ln \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] - kT \ln \mathcal{A}. \quad (68)$$

We should point out that this approximation should only be used in those terms containing the \hbar^2 quantum corrections as it is based on the equilibrium Wigner distribution function. We can neglect the second term since this gives a contribution of order \hbar^4 in $\tilde{\mathcal{E}}_{eff}$ and \tilde{D}_{eff} . We can also neglect the last term in derivatives of V for uniform T and nondegenerate semiconductors. Thus,

$$\nabla^2 V(\vec{q}) = -kT \nabla^2 \ln n. \quad (69)$$

We rewrite $\tilde{\mathcal{E}}_{eff}$ and \tilde{D}_{eff} as

$$e\tilde{\mathcal{E}}_{eff} = \nabla \left\{ V(q) + m^* v^2 - \frac{\hbar^2}{24m^*} \nabla^2 \ln n - \frac{\hbar^2}{12kT} (\nabla^2 \ln n) v^2 - \frac{\hbar^2 m^*}{24(kT)^2} (\nabla^2 \ln n) v^4 \right\}, \quad (70)$$

$$\tilde{D}_{eff} = \frac{\mu}{e} \left\{ kT + m^* v^2 - \frac{\hbar^2}{24m^*} \nabla^2 \ln n - \frac{\hbar^2}{12kT} (\nabla^2 \ln n) v^2 - \frac{\hbar^2 m^*}{24(kT)^2} (\nabla^2 \ln n) v^4 \right\}. \quad (71)$$

Thus, quantum corrections to the semiconductor drift-diffusion equation result in explicitly renormalizing the total drift force and the ‘‘diffusion constant.’’ These are nonequilibrium concepts appropriate to transport problems. This leads us to the important concept of quantum diffusion correction, not fully appreciated in previous formulations focused on stationary concepts of energy and stress tensor. Thus, aside from the quantum potential correction, we have also explicitly taken into account the quantum diffusion correction. These equations together with the Poisson equation for the potential Φ , constitute the QDD equation that is expected to serve as a fast quantum-transport solver for emerging nanotransistors and heterojunction devices. These results can readily be extended to 3D. In 3D, including a given variation $T(\mathbf{q})$, we write the QDD equations as

$$\frac{\partial}{\partial t} n = -\nabla \cdot \mathbf{n} \mathbf{v}, \quad (72)$$

$$\mathbf{J} = -en\mathbf{v} = e\mu \mathbf{E}_{eff} n + e\tilde{D}_{eff} \nabla n. \quad (73)$$

Here we define

$$e\mathbf{E}_{eff} = \nabla \left\{ V(\mathbf{q}) + kT + m^* \mathbf{v} \cdot \vec{\mathbf{v}} - \frac{\hbar^2}{24m^* kT} \nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} - \frac{\hbar^2}{12(kT)^2} \left(\nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} \right) \mathbf{v} \cdot \mathbf{v} - \frac{\hbar^2 m^*}{24(kT)^3} \left(\nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} \right) |v|^4 \right\}, \quad (74)$$

where we included kT in the potential correction to cover the case of a given variation of $T(\mathbf{q})$. The diffusion coefficient now reads

$$\tilde{D}_{eff} = \frac{\mu}{e} \left\{ kT + m^* \mathbf{v} \cdot \mathbf{v} - \frac{\hbar^2}{24m^* kT} \nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} - \frac{\hbar^2}{12(kT)^2} \left(\nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} \right) \mathbf{v} \cdot \mathbf{v} - \frac{\hbar^2 m^*}{24(kT)^3} \left(\nabla \cdot \nabla kT \ln \frac{n}{\mathcal{A}} \right) |v|^4 \right\}. \quad (75)$$

VII. COMPARISON WITH OTHER RELATED WORKS

A recent paper by Ankerhold *et al.* [19] discusses quantum corrections to the effective potential V_{eff} and diffusion coefficient D_{eff} of a quantum Smoluchowski equation in the context of the path integral technique. The barrier system is considered to be coupled to the heat bath in the strong friction limit at low temperatures. They found that at moderate temperatures, where the thermal fluctuations mask the quantum fluctuations, the influence of the quantum correction in the effective potential prevails, effectively lowering the barrier height. What is more intriguing in their work is that at low temperatures strong effects of quantum fluctuations in the diffusion coefficient are revealed.

Our drift-diffusion equations, which correspond to their Smoluchowski equation, agree with their result in that the leading corrections to the effective potential and diffusion coefficient involve the second derivative of the potential. Our results differ in the measurement scale of the quantum correction used. Ankerhold *et al.* use the quantum fluctuation in the position coordinates, namely, $\langle q^2 \rangle - \langle q^2 \rangle_{cl}$, which is a function of \hbar and damping constant, but also goes to zero in the limit as $\hbar \rightarrow 0$. The corresponding classical problem to the one considered by Ankerhold *et al.* is the classic Kramer’s problem of Brownian motion over a potential barrier [20], whereas we are interested in the motion of Fermi-Dirac particles in semiconductor heterojunction nanostructures under an arbitrary bias. Since the typical solution for the stationary current of the drift-diffusion equations depends exponentially on the potential and temperature, it is also expected that the quantum-corrected stationary current will depend exponentially on the effective potential and quantum fluctuations. This would also mean that the escape rate over the barrier will be strongly dependent on the quantum fluctuations, as was indeed found by Ankerhold *et al.* The effect of friction in our drift-diffusion equations is incorporated in the mobility parameter μ , and depends arbitrarily on the strength of the scattering or friction. This parameter arises from the relaxation time or mean free path approximation to the collision term in Eq. (2), which can be rigorously derived from the nonequilibrium quantum field theoretical Green’s function technique for Fermi-Dirac particles [7,8]. Indeed, in the absence of quantum corrections near equilibrium, our effective diffusion coefficient satisfies the Einstein relation.

Several other papers, although directly related to the present work, do not discuss the quantum correction to the diffusion coefficient at all but instead focus on the calculation of the smooth effective classical potential in QHD by

employing the path integral technique of Feynman and Kleinert [21] using a Boltzmann distribution. Gardner's later work and that of others [22] exemplify this type of effort. From our viewpoint, there are really two separate issues to be resolved; the first can be characterized as numerical, and the second issue is fundamental and physical. These issues are (a) the treatment of the abrupt potential in heterojunction semiconductor devices, and (b) the correct quantum nonlinearity capable of approximating quantum coherence in resonant tunneling structures (RTS's). The first arises because of the presence of higher-order derivatives of the classical potential occurring in the quantum corrections. We feel that the second issue is crucial to the foundation of QHD and QDD as viable tools for providing a fast quantum transport solver for nanodevices. This quantum coherence is manifested, both experimentally and through numerical simulation of Eq. (2) [9,23], by the highly nonlinear current-voltage (I - V) characteristics of RTS's. Roughly, the I - V characteristic is given by $I = C_1 V \theta(V_p - V) + C_2 (V - V_p) \theta(V - V_p)$, where $\theta(V - V_p)$ is a step function and V_p corresponds to the current peak or resonant current voltage. Thus, the I - V characteristic is highly nonlinear, exhibiting a resonant peak and fast current collapse after resonance, and generally showing a significant peak-to-valley ratio at low temperatures. A detailed discussion of the physics of resonant tunneling structures is given by Buot *et al.* [23]. We feel that we have given in this paper the important nonequilibrium quantum nonlinearity capable of approximating the highly nonlinear I - V characteristic of resonant tunneling nanodevices. In the high-temperature limit, where the Fermi-Dirac distribution goes into the Boltzmann distribution, then the use of the Feynman-Kleinert smooth effective classical potential would be advantageous to the numerical implementation. However, there may be other ways to resolve this numerical problem other than the Feynman-Kleinert smoothing procedure.

In view of the use of the Boltzmann distribution in the Wigner method of expanding the Wigner distribution function to $O(\hbar^2)$, several authors restart the derivation by solving the Bloch equation for the density matrix, where the Boltzmann distribution is assumed from the beginning [22]. In this way the connection to the Feynman-Kleinert path integral technique becomes natural, and the resulting QHD equations have a smooth effective classical potential. However, since we are interested in charge carriers in semiconductors obeying Fermi-Dirac statistics, it is clear that the starting point of these formulations assumed that the temperature is high enough for the Fermi-Dirac distribution to turn into a Boltzmann distribution. It should be pointed out that in the direct numerical simulations of Eq. (2) the Fermi-Dirac distribution was always used for the supply of tunneling electrons, yielding results in agreement with experiments [7,9]. Moreover, having a smooth effective classical potential only solves the numerical issue cited above, but not necessarily the fundamental physical issue.

The method used in this paper is based on the rigorous expansion of the free energy to $O(\hbar^2)$ using Fermi-Dirac statistics without the need for a small parameter. Thus, we have given a formulation based on the Fermi-Dirac particle distribution from the beginning, valid for all temperature

ranges, as well as incorporating all important quantum nonlinearities in the form of nonequilibrium quantum corrections not considered before. This quantum nonlinearity is deemed necessary to properly approximate the highly nonlinear resonant tunneling I - V characteristic of RTS's.

VIII. CONCLUDING REMARKS

The analytical results presented in this paper show that the quantum corrections to the Wigner distribution transport equations involve dynamical and nonequilibrium corrections not treated before to our knowledge. These quantum dynamical corrections go to zero in the absence of current and heat flux. The physically meaningful quantum transport corrections are the quantum corrections to the drift force (potential) and diffusion coefficients which are inherently nonequilibrium quantities. This is not at all surprising since quantum mechanics has the properties of both particles and fluctuating fields or waves. The quantum correction to the drift force or potential demonstrates the particle aspect in the sense of the Bohm Hamilton-Jacobi particle formulation of quantum mechanics, whereas the quantum correction to the diffusion coefficients demonstrates the fluctuating field aspect in the sense of the stochastic formulation of quantum mechanics initiated by Nelson [18] and supported by the recent work of Ankerhold *et al.* [19]. In fact, quantum diffusion is at the heart of the localization/delocalization theory of Anderson [24].

The "spectral" aspect of our approach lies in the use of the Hermite polynomial expansion of the nonequilibrium distribution function in phase space which allows us to establish the exact nature of the quantum hierarchy in real space, inherent in the exact Wigner transport equation in phase space. This is coupled with the use of the Buot formula for $\text{Tr } \mathcal{H}^n$ to obtain the equilibrium Wigner distribution function solution as an expansion in powers of \hbar^2 . This avoids the need for a rather restrictive assumption based on a perturbative expansion in terms of a small parameter which was originally done by Wigner [15]. Thus, our approach eliminates the conceptual difficulty of applying the QHD and QDD equations to strongly varying potentials in heterojunction devices where the small parameter used by Wigner is not valid. Moreover, the use of the Hermite polynomial expansion enables us to microscopically examine the equations for the various moments in the decoupling procedure. It allows us to account for the contribution of higher-order moments to the solution of the lower-order moments.

ACKNOWLEDGMENTS

One of the authors (F.A.B.) is grateful to Dr. Andrzej Przekwas, CFDRRC, and Professor Edwin Kan and Venkat Narayanan, Cornell University, for stimulating discussions and for drawing his attention to the urgent need for a fast multidimensional quantum transport solver. This work was performed during F.A.B.'s stay at CFDRRC while on sabbatical leave from the U.S. Naval Research Laboratory. This work is partly funded by DARPA. He is thankful to Dr. A. Przekwas and Dr. A. Singhal for their hospitality at CFDRRC.

APPENDIX A: EXPANSION OF WIGNER DISTRIBUTION FUNCTION TO $O(\hbar^2)$

Upon expanding the cosine function to $O(\hbar^2)$ in Eq. (18), we obtain the Buot general formula for the trace of any operator raised to any power n . Thus, $\text{Tr } \mathcal{K}^n$ is given by

$$\begin{aligned}
\text{Tr } \mathcal{K}^n = & (N\hbar^3)^{-1} \text{Tr}_{\text{band}} \sum_{\vec{p}, \vec{q}} \left\{ [K(\vec{p}, \vec{q})]^n - \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 \left[\frac{(n-1)(n-2)}{2} [K(\vec{p}, \vec{q})]^{n-2} \left(\left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \odot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \right\} \right. \right. \right. \\
& \left. \left. \left. - \left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{q}} \odot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{p}} \right\} \right) \right] + \left(\frac{(n-1)(n-2)(n-3)}{6} - \frac{(n-1)(n-2)}{2} \right) \right. \\
& \times [K(\vec{p}, \vec{q})]^{n-3} \left(\left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \odot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \right\} + \left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \odot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \right\} \right. \\
& \left. \left. - \left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{q}} \odot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \right\} - \left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{p}} \odot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \right\} \right) + 2 \left(\frac{(n)(n-1)(n-2)}{6} - \frac{(n-1)(n-2)}{2} \right) \\
& \times [K(\vec{p}, \vec{q})]^{n-3} \left(\frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{p}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} + \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} - \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \right. \\
& \left. \left. - \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \right) \right] + O(\hbar^4) \Big\}, \tag{A1}
\end{aligned}$$

where $\{\odot\}$ is a symmetrized tensor contraction, i.e.,

$$\left\{ \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \odot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \right\} \equiv \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial p_i \partial p_j} \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial q_i \partial q_j} + \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial q_i \partial q_j} \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial p_i \partial p_j}, \tag{A2}$$

and use is made of the Einstein convention where repeated indices are summed over. In evaluating the summation as an integral, $(N\hbar^3)^{-1} \sum_{\vec{p}, \vec{q}} \Rightarrow \hbar^{-3} \int d^3 p d^3 q$.

For treating the valence band transport of some semiconductors like GaN, the 6×6 matrix nature of the valence band in $K(\vec{p}, \vec{q})$ may have to be accounted for in evaluating Eq. (A1). For most systems of interest in semiconductor transport physics, we can simplify Eq. (A1) by assuming that $K(\vec{p}, \vec{q})$ is a diagonal matrix. For the case where $K(\vec{p}, \vec{q})$ is diagonal in band index, Eq. (A1) can readily be evaluated to yield

$$\begin{aligned}
\text{Tr } \mathcal{K}^n = & \text{Tr}_{\text{band}} \hbar^{-3} \int d^3 p d^3 q \left\{ [K(\vec{p}, \vec{q})]^n - \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 [K(\vec{p}, \vec{q})]^{n-2} (n-1)(n-2) \right. \\
& \times \left(\frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} - \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{q}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{p}} \right) - \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 [K(\vec{p}, \vec{q})]^{n-3} \frac{(n-1)(n-2)(n-3)}{3} \\
& \times \left(\frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} + \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} - 2 \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} \right) + O(\hbar^4) \Big\}, \tag{A3}
\end{aligned}$$

where the double-dot product indicates tensor contraction,

$$\frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \equiv \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial p_i \partial p_j} \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial q_i \partial q_j}, \tag{A4}$$

using the Einstein convention for the repeated indices. We should point out here that in

$$K(\vec{p}, \vec{q}) = H(\vec{p}, \vec{q}) - \varepsilon_F = E_\lambda \left(\vec{p} - \frac{e\vec{A}}{c} \right) + V(\vec{q}) - \varepsilon_F,$$

$E_\lambda(\vec{p} - e\vec{A}/c)$ is the full energy-band function, by \vec{p} replaced with $\vec{p} - e\vec{A}/c$ in the presence of a magnetic field. The $[K(\vec{p}, \vec{q})]^{n-3}$ terms in Eq. (A3) can be reduced to $[K(\vec{p}, \vec{q})]^{n-2}$ terms, plus terms which are gradient with respect to \vec{p} and \vec{q} in the absence of a magnetic field. In the effective-mass approximation, and in the absence of the magnetic field, Eq. (A3) reduces to

$$\begin{aligned} \text{Tr } \mathcal{K}^n = & \text{Tr}_{\text{band}} h^{-3} \int d^3 p d^3 q \left\{ [K(\vec{p}, \vec{q})]^n - \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 \frac{n(n-1)}{3} [K(\vec{p}, \vec{q})]^{n-2} \left(\frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} : \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \right) \right. \\ & - \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 \frac{n(n-1)}{3} \left(\frac{\partial}{\partial \vec{q}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} [K(\vec{p}, \vec{q})]^{n-2} + \frac{\partial}{\partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} [K(\vec{p}, \vec{q})]^{n-2} \right) \\ & \left. + \frac{1}{2!} \left(\frac{\hbar}{2} \right)^2 (n-1) \left(\frac{\partial}{\partial \vec{q}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{p} \partial \vec{p}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{q}} [K(\vec{p}, \vec{q})]^{n-2} + \frac{\partial}{\partial \vec{p}} \cdot \frac{\partial^2 K(\vec{p}, \vec{q})}{\partial \vec{q} \partial \vec{q}} \cdot \frac{\partial K(\vec{p}, \vec{q})}{\partial \vec{p}} [K(\vec{p}, \vec{q})]^{n-2} \right) + O(\hbar^4) \right\}. \end{aligned} \quad (\text{A5})$$

Therefore, using Eq. (19), it follows that the expression for the Wigner distribution function to $O(\hbar^2)$ is given by Eq. (21).

APPENDIX B: DERIVATION FOR $f_3^w(q, t)$ IN TERMS OF THE MOMENTS AND $f_0^{FD}(q, t)$

We need the third-order Hermite polynomial coefficient in the equation for $(\partial/\partial t)W(q, t)$ which can be determined from Eq. (26):

$$f_3^w(q, t) = \left[1 - \frac{A}{8} + \frac{B}{24} + 7 \frac{CkT}{24} + \frac{C}{24m^*} u^2 \right] f_3^{FD}(q, t) + \frac{CkT}{24} [f_1^{FD}(q, t) + 20f_5^{FD}(q, t)] - \frac{C}{12} \sqrt{\frac{kT}{m^*}} u [f_2^{FD}(q, t) + 4f_4^{FD}(q, t)]. \quad (\text{B1})$$

The Fermi-Dirac Hermite coefficients $f_4^{FD}(q, t)$ and $f_5^{FD}(q, t)$ are evaluated in Appendixes B and C, respectively. Substituting in terms of the moments and $f_0^{FD}(q, t)$, we obtain

$$\begin{aligned} 2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_3^w(q, t) = & \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] \left\{ \frac{2}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{\text{heat flux}}}{kT} + \frac{1}{3!} \rho(q, t) \frac{u^3(q, t)}{(\sqrt{m^* kT})^3} \right\} \\ & + \left\{ \frac{2}{24} C \sqrt{\frac{m^*}{kT}} Q_{\text{heat flux}} + \frac{\rho(q, t)}{24} \frac{C}{m^*} \frac{u^3(q, t)}{(\sqrt{m^* kT})} \right\} + \left\{ \frac{1}{3} \frac{C}{24m^*} \sqrt{\frac{m^*}{kT}} \frac{Q_{\text{heat flux}}}{kT} u^2 \right. \\ & \left. + \frac{1}{6} \rho(q, t) \frac{C}{24m^*} \frac{u^5(q, t)}{(\sqrt{m^* kT})^3} \right\} + \frac{C}{24} \sqrt{\frac{kT}{m^*}} \rho(q, t) u + \left\{ \frac{1}{6(24)} CkT \rho(q, t) \right. \\ & - \frac{5u}{3(24)\sqrt{m^* kT}} CkT \rho(q, t) - \frac{u^3(q, t)}{3(24)(\sqrt{m^* kT})m^*} C \rho(q, t) - \frac{10}{3(24)} C \sqrt{\frac{m^*}{kT}} Q_{\text{heat flux}} \\ & \left. + \frac{3}{2} \frac{C}{24} \sqrt{\frac{m^*}{kT}} \frac{Q_{\text{heat flux}}}{kT} \frac{u^2}{m^*} + \frac{C}{24m^{*2}} \frac{u^5}{6\sqrt{m^* kT}(kT)} \rho(q, t) \right\} - \frac{C}{12} \sqrt{\frac{kT}{m^*}} \frac{\rho(q, t) u^3}{2m^* kT} \\ & - \frac{C}{12} \frac{5}{3} \sqrt{\frac{m^*}{kT}} \frac{Q_{\text{heat flux}}}{kT} \frac{u^2}{m^*} - \frac{u^3}{3(12)\sqrt{m^* kT}m^*} C \rho(q, t) - \frac{C}{12m^{*2}} \frac{u^5}{3\sqrt{m^* kT}kT} \rho(q, t) \\ & \left. + \frac{C}{(12)6} \sqrt{\frac{kT}{m^*}} \rho(q, t) u. \right\} \quad (\text{B2}) \end{aligned}$$

Collecting terms, we end up with

$$\begin{aligned}
2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_3^w(q,t) &= \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] \rho(q,t) \frac{2}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{\rho(q,t)kT} + \frac{1}{3!} \left[1 - \frac{A}{8} + \frac{B}{24} + \frac{CkT}{24} \right] \rho(q,t) \frac{u^3(q,t)}{(\sqrt{m^* kT})^3} \\
&+ \frac{1}{6(24)} CkT \rho(q,t) - \frac{4}{3(24)} C \sqrt{\frac{m^*}{kT}} Q_{heat\ flux} - \frac{1}{3(24)} \sqrt{\frac{kT}{m^*}} C \rho(q,t) u \\
&- \frac{3}{2} \frac{C}{24} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{kT} \frac{u^2}{m^*} - \frac{C}{12} \sqrt{\frac{kT}{m^*}} \frac{\rho(q,t)u^3}{2m^*kT} - \frac{1}{3} \rho(q,t) \frac{C}{24m^*} \frac{u^5(q,t)}{(\sqrt{m^* kT})^3}. \tag{B3}
\end{aligned}$$

APPENDIX C: DERIVATION FOR $f_4^{FD}(q,t)$ IN TERMS OF THE MOMENTS AND $f_0^{FD}(q,t)$

We need the fourth-order Hermite polynomial, namely,

$$\langle \tilde{H}_4(p) \rangle \equiv \langle He_4(\xi) \rangle = \left\langle \left(\frac{p}{\sqrt{m^* kT}} \right)^4 \right\rangle - \left\langle 6 \left(\frac{p}{\sqrt{m^* kT}} \right)^2 \right\rangle + \langle 3 \rangle = \left\langle \left(\frac{p}{\sqrt{m^* kT}} \right)^4 \right\rangle - 6\tilde{H}_2(p) - 3\tilde{H}_0(p). \tag{C1}$$

Therefore

$$2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_4^{FD}(q,t) = \frac{1}{12} \left\langle \left(\frac{p}{\sqrt{m^* kT}} \right)^4 \right\rangle - \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_2^{FD}(q,t) - \frac{1}{8} 2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_0^{FD}(q,t). \tag{C2}$$

Substituting $p = p' + u$, then

$$\begin{aligned}
\left\langle \left(\frac{p}{\sqrt{m^* kT}} \right)^4 \right\rangle &= \left(\frac{1}{m^* kT} \right)^2 \langle \{ p'^4 + 4p'^3 u + 4p'^2 u^2 + u^4 \} \rangle \\
&= \left\langle \frac{p'^4}{(m^* kT)^2} \right\rangle + \left\langle \frac{[p'^3 + 2p'^2 u + (p'^2 + u^2)u]u}{(m^* kT)^2} \right\rangle + \left\langle \frac{(3p'^3 + p'^2 u)u}{(m^* kT)^2} \right\rangle \tag{C3}
\end{aligned}$$

$$\begin{aligned}
&= \left\langle \frac{p'^4}{(m^* kT)^2} \right\rangle + \frac{2}{(kT)^2} \left\{ Q_{heat\ flux} + W \frac{u}{m^*} + \rho(q,t)kT \frac{u}{m^*} \right\} u + 3 \frac{Q_{heat\ flux}}{(kT)^2} u \\
&+ \frac{\rho(q,t)kT}{(kT)^2} \frac{u^2}{m^*}. \tag{C4}
\end{aligned}$$

Thus we have

$$\begin{aligned}
2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_4^{FD}(q,t) &= \frac{1}{12} \left\langle \frac{p'^4}{(m^* kT)^2} \right\rangle + \frac{2}{(kT)^2} \left\{ Q_{heat\ flux} + W \frac{u}{m^*} + \rho(q,t)kT \frac{u}{m^*} \right\} u + 3 \frac{Q_{heat\ flux}}{(kT)^2} u + \frac{\rho(q,t)kT}{(kT)^2} \frac{u^2}{m^*} \\
&- \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_2^{FD}(q,t) - \frac{1}{8} 2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_0^{FD}(q,t), \tag{C5}
\end{aligned}$$

$$\begin{aligned}
2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_4^{FD}(q,t) &= \left\{ \frac{1}{12} \left\langle \frac{p'^4}{(m^* kT)^2} \right\rangle + \left[\frac{1}{12} \frac{2}{(kT)^2} Q_{heat\ flux} + \frac{1}{12} \left(\frac{\rho(q,t)}{kT} + \frac{1}{(kT)^2} \frac{\rho(q,t)u^2}{m^*} \right) \frac{u}{m^*} \right. \right. \\
&+ \left. \frac{1}{12} \frac{2}{(kT)} \rho(q,t) \frac{u}{m^*} \right\} u + 3 \frac{1}{12} \frac{Q_{heat\ flux}}{(kT)^2} u + \frac{1}{12} \frac{\rho(q,t)}{kT} \frac{u^2}{m^*} \left. \right\} - \frac{\rho(q,t)u^2}{4m^* kT} - \frac{1}{8} \rho(q,t), \tag{C6}
\end{aligned}$$

$$2 \frac{(2\pi m^* kT)^{3/2}}{(2\pi\hbar)^3} f_4^{FD}(q,t) = \left\{ \frac{1}{12} \left\langle \frac{p'^4}{(m^* kT)^2} \right\rangle + \frac{5}{12} \frac{Q_{heat\ flux}}{(kT)^2} u + \frac{1}{12} \frac{\rho(q,t)}{kT} \frac{u^2}{m^*} + \frac{1}{12} \frac{1}{(kT)^2} \frac{\rho(q,t)u^4}{m^{*2}} \right\} - \frac{1}{8} \rho(q,t).$$

Dividing by $2[(2\pi m^* kT)^{3/2}/(2\pi\hbar)^3] f_0^{FD}(q,t)$, we thus obtain

$$f_4^{FD}(q,t) = \left[\frac{1}{12\rho(q,t)} \left\langle \frac{p'^4}{(m^*kT)^2} \right\rangle + \frac{5}{12} \frac{Q_{heat\ flux}}{\rho(q,t)(kT)^2} u + \frac{1}{12} \frac{1}{kT} \frac{u^2}{m^*} + \frac{1}{12} \frac{1}{(kT)^2} \frac{u^4}{m^{*2}} - \frac{1}{8} \right] f_0^{FD}(q,t). \quad (C7)$$

If we simply approximate the fourth-order moment of the random fluctuation in $\langle p'^4/(m^*kT)^2 \rangle$ by $4\rho(q,t)(kT)^2/4(kT)^2$, then we have

$$f_4^{FD}(q,t) = \left[\frac{5}{12} \frac{Q_{heat\ flux}}{\rho(q,t)(kT)^2} u + \frac{1}{12} \frac{1}{kT} \frac{u^2}{m^*} + \frac{1}{12} \frac{1}{(kT)^2} \frac{u^4}{m^{*2}} - \frac{1}{24} \right] f_0^{FD}(q,t). \quad (C8)$$

APPENDIX D: DERIVATION FOR $f_5^{FD}(q,t)$ IN TERMS OF THE MOMENTS AND $f_0^{FD}(q,t)$

We have

$$\begin{aligned} \langle \tilde{H}_5(p) \rangle &\equiv \langle H e_5(\xi) \rangle = \xi^5 - 10\xi^3 + 15\xi \\ &= \left\langle \left(\frac{p}{\sqrt{m^*kT}} \right)^5 \right\rangle - \left\langle 10 \left(\frac{p}{\sqrt{m^*kT}} \right)^3 \right\rangle + \left\langle 15 \left(\frac{p}{\sqrt{m^*kT}} \right) \right\rangle = \left\langle \left(\frac{p}{\sqrt{m^*kT}} \right)^5 \right\rangle - \langle 10\tilde{H}_3(p) \rangle - \langle 15\tilde{H}_1(p) \rangle. \end{aligned} \quad (D1)$$

Therefore

$$2 \frac{(2\pi m^*kT)^{3/2}}{(2\pi\hbar)^3} f_5^{FD}(q,t) = \frac{1}{120} \left\langle \left(\frac{p}{\sqrt{m^*kT}} \right)^5 \right\rangle - \frac{(2\pi m^*kT)^{3/2}}{(2\pi\hbar)^3} f_3^{FD}(q,t) - \frac{1}{4} \frac{(2\pi m^*kT)^{3/2}}{(2\pi\hbar)^3} f_1^{FD}(q,t). \quad (D2)$$

Substituting $p = p' + u$,

$$\begin{aligned} \left\langle \left(\frac{p}{\sqrt{m^*kT}} \right)^5 \right\rangle &= \frac{1}{\sqrt{m^*kT}} \left(\frac{1}{m^*kT} \right)^2 \langle \{p'^5 + 5p'^4u + 8p'^3u^2 + 8p'^2u^3 + 5p'u^4 + u^5\} \rangle \\ &= \frac{1}{\sqrt{m^*kT}} \left(\frac{1}{m^*kT} \right)^2 \langle \{p'^5 + 5p'^4u + 8p'^3u^2 + 8p'^2u^3 + u^5\} \rangle = \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle \\ &\quad + \left\langle \frac{[p'^3 + 2p'^2u + (p'^2 + u^2)u]u^2}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \left\langle \frac{(5p'^4 + 7p'^3u + 5p'^2u^2)u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle \\ &= \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\sqrt{m^*kT}(kT)^2} \left\{ 2Q_{heat\ flux} + 2W \frac{u}{m^*} + 2\rho(q,t)kT \frac{u}{m^*} \right\} u^2 + \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle \\ &\quad + 7 \frac{Q_{heat\ flux}}{\sqrt{m^*kT}(kT)^2} u^2 + \frac{5\rho(q,t)kT}{\sqrt{m^*kT}(kT)^2} \frac{u^3}{m^*} \end{aligned} \quad (D3)$$

$$= \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\sqrt{m^*kT}(kT)^2} \left\{ 9Q_{heat\ flux} + 2W \frac{u}{m^*} + 7\rho(q,t)kT \frac{u}{m^*} \right\} u^2. \quad (D4)$$

Thus, we have

$$\begin{aligned} 2 \frac{(2\pi m^*kT)^{3/2}}{(2\pi\hbar)^3} f_5^{FD}(q,t) &= \frac{1}{120} \left\{ \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\sqrt{m^*kT}(kT)^2} \left\{ 9Q_{heat\ flux} + 2W \frac{u}{m^*} \right. \right. \\ &\quad \left. \left. + 7\rho(q,t)kT \frac{u}{m^*} \right\} u^2 \right\} - \left\{ \frac{1}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{kT} + \frac{1}{3!} \rho(q,t) \frac{u^3(q,t)}{2(\sqrt{m^*kT})^3} \right\} - \frac{1}{4} \rho(q,t) \frac{u}{2\sqrt{m^*kT}}. \end{aligned}$$

Dividing by $2[(2\pi m^*kT)^{3/2}/(2\pi\hbar)^3]f_0^{FD}(q,t)$, we thus obtain

$$f_5^{FD}(q,t) = \frac{1}{120} \left\{ \frac{1}{\rho(q,t)} \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\rho(q,t)} \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\sqrt{m^*kT}(kT)^2} \left[9 \frac{Q_{heat\ flux}}{\rho(q,t)} + 2 \frac{W}{\rho(q,t)} \frac{u}{m^*} + 7kT \frac{u}{m^*} \right] u^2 \right\} f_0^{FD}(q,t) - \left\{ \frac{1}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{\rho(q,t)kT} + \frac{1}{3!} \frac{u^3(q,t)}{2(\sqrt{m^*kT})^3} \right\} f_0^{FD}(q,t) - \frac{u}{8\sqrt{m^*kT}} f_0^{FD}(q,t), \quad (D5)$$

$$f_5^{FD}(q,t) = \frac{1}{120} \left\{ \frac{1}{\rho(q,t)} \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\rho(q,t)} \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \left[9 \frac{Q_{heat\ flux}}{\sqrt{m^*kT}(kT)^2\rho(q,t)} u^2 + \left(kT \frac{u^3}{\sqrt{m^*kT}(kT)^2m^*} + \frac{u^5}{\sqrt{m^*kT}(kT)^2m^{*2}} \right) + 7kT \frac{u^3}{\sqrt{m^*kT}(kT)^2m^*} \right] \right\} f_0^{FD}(q,t) - \left\{ \frac{1}{3!} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{\rho(q,t)kT} + \frac{1}{3!} \frac{u^3(q,t)}{2(\sqrt{m^*kT})^3} \right\} f_0^{FD}(q,t) - \frac{u}{8\sqrt{m^*kT}} f_0^{FD}(q,t), \quad (D6)$$

$$f_5^{FD}(q,t) = \frac{1}{120} \left\{ \frac{1}{\rho(q,t)} \left\langle \frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \frac{1}{\rho(q,t)} \left\langle \frac{5p'^4u}{\sqrt{m^*kT}(m^*kT)^2} \right\rangle + \left[9 \frac{Q_{heat\ flux}}{\sqrt{m^*kT}(kT)^2\rho(q,t)} u^2 + \frac{u^5}{\sqrt{m^*kT}(kT)^2m^{*2}} \right] \right\} f_0^{FD}(q,t) - \frac{1}{6} \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{\rho(q,t)kT} f_0^{FD}(q,t) - \frac{u^3(q,t)}{60(\sqrt{m^*kT})m^*kT} f_0^{FD}(q,t) - \frac{u}{8\sqrt{m^*kT}} f_0^{FD}(q,t). \quad (D7)$$

Again we make the following approximations:

$$\left\langle \frac{p'^4}{(m^*kT)^2} \right\rangle \approx \frac{4\rho(q,t)(kT)^2}{4(kT)^2},$$

$$\frac{p'^5}{\sqrt{m^*kT}(m^*kT)^2} \approx \frac{\sqrt{m^*kT}4\rho(q,t)(kT)^2}{\sqrt{m^*kT}4(kT)^2}. \quad (D8)$$

Then we obtain

$$f_5^{FD}(q,t) = \left\{ \frac{1}{120} - \frac{u}{12\sqrt{m^*kT}} - \frac{u^3(q,t)}{60(\sqrt{m^*kT})m^*kT} - \left[\frac{1}{6} - \frac{3}{40} \frac{u^2}{kTm^*} \right] \sqrt{\frac{m^*}{kT}} \frac{Q_{heat\ flux}}{\rho(q,t)kT} + \frac{u^5}{120\sqrt{m^*kT}(kT)^2m^{*2}} \right\} f_0^{FD}(q,t). \quad (D9)$$

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