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# Exact Integral Operator Form of the Wigner Distribution-Function Equation in Many-Body Quantum Transport Theory

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A formal derivation of a generalized equation of a Wigner distribution function including all many-body effects and all scattering mechanisms is given. The result is given in integral operator form suitable for application to the numerical modeling of quantum tunneling and quantum interference solid state devices. In the absence of scattering and many-body effects, the result reduces to the "noninteracting-particle" Wigner distribution function equation, often used to simulate resonant tunneling devices. The derivation uses a Weyl transform technique which can easily incorporate Bloch electrons. Weyl transforms of self-energies are derived. Various simplifications of a general quantum transport equation for semiconductor device analysis and self-consistent numerical simulation of a quantum distribution function in the phase-space/frequency–time domain are discussed. Recent attempts to include collisions in the Wigner distribution-function approach to the numerical simulation of tunneling devices are clearly shown to be non-self-consistent and inaccurate; more accurate numerical simulation is needed for a deeper understanding of the effects of collision and scattering.

**KEY WORDS**: Wigner distribution function; Weyl transform; non-equilibrium Green's function technique; quantum distribution function; many-body quantum transport equation; quantum Boltzmann equation; Kadanoff–Baym Ansatz; electron–phonon scatterings.

## 1. INTRODUCTION

Discussions of quantum transport in the literature, starting with the work of Kadanoff and Baym$^{(1)}$ and Keldysh,$^{(2)}$ using the Green's function techni-

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que for dissipative systems initiated by Schwinger,(3) often focus on the derivation of the so-called quantum Boltzmann equation (QBE).(4–6, 24) Although these works give the essential corrections to the classical Boltzmann equation, the resulting equations are not useful for application to resonant tunneling heterostructure devices. The major reason for the lack of usefulness is that these equations are obtained for a slowly varying field in space and time. In heterojunction quantum-based devices, strong nonuniformity in space coupled with very high-frequency operation(7–9) almost always invalidates these assumptions.

In recent years, numerical simulations and device characterizations of resonant-tunneling devices (RTD) have been achieved through the use of the Wigner distribution function equation,(7–10) first written by Wigner more than five decades ago. These numerical simulations have clearly demonstrated the potential of these quantum-based devices for very high frequency operation in the tera hertz range.(7–9) The potential for the practical utilization of these devices, and other quantum-based devices, for commercial and military applications seems unlimited. Moreover, coupling of the quantum transport numerical technique with the self-consistent ensemble particle Monte Carlo technique will further enchance the applicability of transport device physics for modeling novel heterojunction devices. A way to couple accurately ensemble particle Monte Carlo with space- and time-dependent quantum tunneling has recently been advocated by the author(11) via transformation of quantum transport into a "quantum particle trajectory" representation.(9)

The inclusion of many-body effects and scattering/dissipation in the original Wigner distribution function equation, which is essential for a realistic simulation of RTD in the quantum region, has not always been clear in the literature. In most cases, these are done by using analogies to the classical Boltzmann equation or by applying other heuristic arguments(12) and trying out in the computer to see if one gets reasonable results. What is needed for more exact numerical work is an exact formalism for including many-body effects and scatterings in the "non-interacting-particle" Wigner distribution function equation. Any approximation must then be based on an exact formulation in order to define clearly the range of validity of the approximation. To the author's knowledge, an exact formulation of a generalized Wigner distribution function transport equation has not been treated in the literature. What has often been treated is the generalized Boltzmann transport equation (QBE) at very high constant electric field. Because of the highly nonuniform space- and time-dependent field distribution in realistic devices, these types of formulations are not of much help for the numerical work of device physicists.

The purpose of this paper is to present a formal derivation of a generalized Wigner transport equation including all many-body effects and scattering mechanisms, which is useful for numerical work. I use the theory of the nonequilibrium Green's function technique, originally treated by Schwinger,(3) Kadanoff and Baym,(1) and Keldysh.(2) From the equation of motion for the nonequilibrium Green's equations, the so-called quantum Boltzmann equation follows when the assumptions of slow time and space variations in the system are made. With an eye to numerical simulation, I avoid these assumptions and formulate an exact integral form of a generalized Wigner distribution transport equation which immediately gives the conventional Wigner distribution function equation in the limit of vanishing self-energies for nonrelativistic particles. In passing, it is worth noting that all QBE results do not yield the noninteracting "single-particle" Wigner distribution quantum transport equation in the absence of collisions and scatterings.

## 2. NONEQUILIBRIUM GREEN'S FUNCTION FORMALISM

For a nonequilibrium or nonstationary system, where dynamics is dependent on the direction of time, no state of the system in the future may be identified with any state in the past. For this reason, expectation values and Green's functions are defined on a contour in which the time arguments runs from the initial time $t_0$ to the "far" future (e.g., largest time argument of the Green's function) and then back to $t_0$. With this definition, a perturbation expansion of the Green's function along the path is analogous to the conventional many-body equilibrium Green's function expansion and a separation of many-body interaction terms into self-energy parts and single-particle Green's function terms is justified for expectation values defined along this contour.

With time arguments along the contour, the nonequilibrium Green's function is defined as

$$iG(x_1, t_1, x_2, t_2) \equiv \langle \hat{\Psi}_H(x_1, t_1)\, \hat{\Psi}_H^{\dagger}(x_2, t_2) \rangle \tag{1}$$

where the time ordering operator $T$ orders the time argument along the contour. Thus, we may write also

$$G(x_1, t_1, x_2, t_2) = \Theta(t_1, t_2)\, G^{>}(x_1, t_1, x_2, t_2) + \Theta(t_2, t_1)\, G^{<}(x_1, t_1, x_2, t_2) \tag{2}$$

where

$$\begin{aligned} \Theta(t_1, t_2) &= 1 \qquad \text{if} \quad t_1 \text{ is later on a contour than } t_2 \\ &= 0 \qquad \text{if} \quad t_1 \text{ is earlier than } t_2 \end{aligned}$$

Employing Feynman's perturbation expansion method or Schwinger's variational[13] method for introducing the self-energy, we have that the Green's function satisfies integral equations with time arguments defined on the contour in the usual fashion as

$$\oint d2\, G^{-1}_{\alpha\sigma}(1, 2)\, G_{\sigma\beta}(2, 1') = \delta_{\alpha\beta}(1, 1') \tag{3}$$

$$\oint d2\, G_{\alpha\sigma}(1, 2)\, G^{-1}_{\sigma\beta}(2, 1') = \delta_{\alpha\beta}(1, 1') \tag{4}$$

Separating the self-energy, we have

$$\oint d2\, G^{0^{-1}}_{\alpha\sigma}(1, 2')\, G_{\sigma\beta}(2, 1') = \delta_{\alpha\beta}(1, 1') + \oint d2\, \Sigma_{\alpha\sigma}(1, 2)\, G_{\sigma\beta}(2, 1') \tag{5}$$

$$\oint d2\, G_{\alpha\sigma}(1, 2)\, G^{0^{-1}}_{\sigma\beta}(2, 1') = \delta_{\alpha\beta}(1, 1') + \oint d2\, G_{\alpha\sigma}(1, 2)\, \Sigma_{\sigma\beta}(2, 1) \tag{6}$$

where

$$G^{0^{-1}}_{\alpha\sigma}(1, 2) = \left[ -\frac{\hbar}{i}\frac{\partial}{\partial t_1} - E_\alpha\left( -\frac{\hbar}{i}\nabla_1 \right) \right] \delta_{\alpha\sigma}(1, 2) \tag{7}$$

The last two equations give the equations of motion obeyed by the Green's function

$$\begin{aligned} &\left[ -\frac{\hbar}{i}\frac{\partial}{\partial t_1} - E_\alpha\left( -\frac{\hbar}{i}\nabla_1 \right) \right] G_{\alpha\beta}(1, 1') \\ &\qquad = \delta_{\alpha\beta}(1, 1') + \oint d2\, \Sigma_{\alpha\sigma}(1, 2)\, G_{\sigma\beta}(2, 1') \end{aligned} \tag{8}$$

$$\begin{aligned} &\left[ \frac{\hbar}{i}\frac{\partial}{\partial t_{1'}} - E_\alpha\left( \frac{\hbar}{i}\nabla_{1'} \right) \right] G_{\alpha\beta}(1, 1') \\ &\qquad = \delta_{\alpha\beta}(1, 1') + \oint d2\, G_{\alpha\sigma}(1, 2)\, \Sigma_{\sigma\beta}(2, 1') \end{aligned} \tag{9}$$

which correspond to the well-known Dyson equations,

$$G_{\alpha\beta}(1, 1') = G^0_{\alpha\beta}(1, 1') + \oint d2 \oint d3\, G^0_{\alpha\sigma}(1, 2)\, \Sigma_{\sigma\eta}(2, 3)\, G_{\eta\beta}(3, 1') \tag{10}$$

$$G_{\alpha\beta}(1, 1') = G^0_{\alpha\beta}(1, 1') + \oint d2 \oint d3\, G_{\alpha\sigma}(1, 2)\, \Sigma_{\sigma\eta}(2, 3)\, G^0_{\eta\beta}(3, 1') \tag{11}$$

In the above equations, $E_\alpha(k)$ is the energy band function for band index $\alpha$, time integration is along the contour, and the Einstein summation convention for the Greek indices is used. The "self-energy" $\Sigma$ has the following general form$^{(13,14)}$:

$$\Sigma_{\alpha\beta}(1,2) = \delta(t_1, t_2)\, \Sigma^{\mathrm{VHF}}_{\alpha\beta}(x_1, x_2, t_1) + \theta(t_1, t_2) \Sigma^{>}_{\alpha\beta}(1,2) + \theta(t_2, t_1)\, \Sigma^{<}_{\alpha\beta}(1,2) \tag{12}$$

where

$$\Sigma^{\mathrm{VHF}} = V(\mathbf{x}_1)\, \delta_{\alpha\beta}(1,1') + \Sigma^{\mathrm{HF}}_{\alpha\beta}(x_1, x_1', t_1) \tag{13}$$

and $V(\mathbf{x}_1)$ is the external potential and $\Sigma^{\mathrm{HF}}_{\alpha\beta}(x_1, x_1, t_1)$ is the Hartree–Fock approximation to the self-energy.

For simplicity in what follows we will consider only a one-band model and drop the Greek indices altogether. However, the inclusion of multiband indices is straightforward and the treatment is analogous to the method given by Korenman$^{(15)}$ in his work on gas lasers. For deriving the quantum transport equation, we are interested in the equations for $G^{<}(x_1, t_1, x_2, t_2)$, which is related to the particle densities. These are obtained from Eqs. (8) and (9) by fixing the order of the time arguments in the Green's functions. From Eq. (8), we have

$$\begin{aligned} &\left[-\frac{\hbar}{i}\frac{\partial}{\partial t_1} - E_\alpha\left(-\frac{\hbar}{i}\nabla_1\right)\right] G^{\lesseqgtr}(1,1') \\ &\quad = \int dx_2\, \Sigma^{\mathrm{VHF}}(x_1, x_2, t_1)\, G^{\gtrless}(x_2, t_2, 1') \\ &\qquad + \int_{t_0}^{t_1} d2\, [\Sigma^{>}(1,2) - \Sigma^{<}(1,2)]\, G^{\gtrless}(2,1') \\ &\qquad + \int_{t_{1'}}^{t_0} d2\, \Sigma^{\gtrless}(1,2)[G^{>}(2,1') - G^{<}(2,1')] \end{aligned} \tag{14}$$

which corresponds to Eqs. (8.27a) and (8.27b) of Kadanoff and Baym,$^{(1)}$ where the expectation values are taken with respect to the equilibrium density operator, which in the limit $t_0 \to -\infty$ gives the same results. From Eq. (9), we have

$$\begin{aligned} &\left[\frac{\hbar}{i}\frac{\partial}{\partial t_{1'}} - E_\alpha\left(-\frac{\hbar}{i}\nabla_{1'}\right)\right] G^{\gtrless}(1,1') \\ &\quad = \int dx_2\, G^{\gtrless}(1, x_2, t_{1'})\, \Sigma^{\mathrm{VHF}}(x_2, x_1, t_{1'}) \\ &\qquad + \int_{t_0}^{t_1} d2\, [G^{>}(1,2) - G^{<}(1,2)]\, \Sigma^{\gtrless}(2,1') \\ &\qquad + \int_{t_{1'}}^{t_0} d2\, G^{\gtrless}(1,2)[\Sigma^{>}(2,1') - \Sigma^{<}(2,1')] \end{aligned} \tag{15}$$

which corresponds to Eqs. (8.28a) and (8.28b) of Kadanoff and Baym.(1) To transform the above equations into representation-independent equations, in the limit $t_0 \to -\infty$, we need to defined advanced and retarded functions on the real-time axis (*i.e.*, not on the contour) for the Green's functions and self-energy functions. For arbitrary double-argument functions in space-time, we define

$$F^r(1, 2) = \theta(t_1 - t_2)[F^>(1, 2) - (F^<(1, 2)] \tag{16}$$

$$F^a(1, 2) = -\theta(t_2 - t_1)[F^>(1, 2) - F^<(1, 2)] \tag{17}$$

These "unequal-time" functions essentially describe the propagation of particles. Therefore, using the above definition of retarded and advanced functions, we can write Eqs. (14) and (15) as follows:

$$-\frac{\hbar}{i}\frac{\partial}{\partial t_1} G^{\gtrless}(1, 1') = \mathscr{H} G^{\gtrless} + \Sigma^r G^{\gtrless} + \Sigma^{\gtrless} G^a \tag{14a}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial t_{1'}} G^{\gtrless}(1, 1') = G^{\gtrless} \mathscr{H} + G^r \Sigma^{\gtrless} + G^{\gtrless} \Sigma^a \tag{15a}$$

where

$$\mathscr{H}(1, 2) = \left[E_\alpha\left(-\frac{\hbar}{i}\nabla_1\right) + V(1)\right]\delta(1 - 2) + \delta(t_1 - t_2)\,\Sigma^{\mathrm{HF}}(x_1, x_2, t_1) \tag{18}$$

The inclusion of the exchange term introduces nonlocality in space in the effective potential included in $\mathscr{H}$. Essentially $\mathscr{H}$ incorporates the dynamical properties of the particles, whereas terms involving $\Sigma^{\gtrless}$ describe the scatterings.

In order to obtain the time evolution equation for the densities, first we have to subtract Eq. (15a) from Eq. (14a), which yields coupled equations for $G^<$ and $G^>$,

$$\begin{aligned} &-\frac{\hbar}{i}\left(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_{1'}}\right) G^{\gtrless}(1, 1') \\ &\qquad = [\mathscr{H}, G^{\gtrless}] + \Sigma^r G^{\gtrless} - G^r \Sigma^{\gtrless} + \Sigma^{\gtrless} G^a - G^{\gtrless} \Sigma^a \end{aligned} \tag{19}$$

which can be written in entirely representation-independent form as

$$[G^{0-1} - \Sigma^\delta, G^{\gtrless}] = (\Sigma^r G^{\gtrless} + \Sigma^{\gtrless} G^a) - (G^r \Sigma^{\gtrless} + G^{\gtrless} \Sigma^a) \tag{20}$$

where

$$\Sigma^\delta(1, 1') = \delta(1, 1')\, V(1) + \delta(t_1 - t_{1'})\,\Sigma^{\mathrm{HF}}(x_1, x_{1'}, t_1) \tag{21}$$

Square bracket indicate commutation of terms separated by a comma. It is easy to show that Eq. (20) can also be written in the following form:

$$[G^{0-1} - \Sigma^{\delta}, G^{\gtrless}] = \tfrac{1}{2}\{(\Sigma^{r} - \Sigma^{a}), G^{\gtrless}\} + \tfrac{1}{2}[(\Sigma^{r} + \Sigma^{a}), G^{\gtrless}] + \tfrac{1}{2}[\Sigma^{\gtrless}, (G^{r} + G^{a})] - \tfrac{1}{2}\{\Sigma^{\gtrless}, G^{r} - G^{a}\} \quad (22)$$

which is the result obtained by Langreth and Wilkins(16) using the analytic continuation procedure of Kadanoff and Baym.(1) The curly brackets in Eq. (22) indicate the anticommutation operation of terms separated by a comma.

We note that the self-energies and Green's functions obey the Hermitian relations

$$[iF(1,2)]^{\dagger} = iF(1,2) \quad (23)$$

$$[iF^{\gtrless}(1,2)]^{\dagger} = iF^{\gtrless}(1,2) \quad (24)$$

$$[F^{r}(1,2)]^{\dagger} = F^{a}(1,2) \quad (25)$$

Indeed, for the "fixed-time order" Green's functions we have, for example,

$$\begin{aligned} G^{<}(1,2)^{\dagger} &= G^{<*}(2,1) \\ &= i\langle \psi_H^{\dagger}(1)\, \psi_H(2)\rangle^{*} \\ &= -i\langle \psi_H^{\dagger}(2)\, \psi_H(1)\rangle \\ &= -G^{<}(1,2) \end{aligned} \quad (26)$$

Therefore, we have $[iG^{<}(1,2)]^{\dagger} = iG^{<}(1,2)$, *i.e.*, $iG^{<}(1,2)$ is self-adjoint, which is the reason why Kadanoff and Baym(1) like to multiply the Green's functions by $i$ when taking their "Fourier transform in relative coordinates," since the results are real quantities.

From Eq. (25) we can define Hermitian functions,

$$\operatorname{Re} F^{r}(1,2) = \frac{1}{2}\,[F^{r}(1,2) + F^{a}(1,2)] \quad (27)$$

$$[\operatorname{Re} F^{r}(1,2)]^{\dagger} = \operatorname{Re} F^{r}(1,2) \quad (28)$$

$$\operatorname{Im} F^{r}(1,2) = \frac{1}{2i}\,[F^{r}(1,2) - F^{a}(1,2)] \quad (29)$$

$$[\operatorname{Im} F^{r}(1,2)]^{\dagger} = \operatorname{Im} F^{r}(1,2) \quad (30)$$

The significance of the above definitions stems from an important result that the Weyl transform(17) (more will be said about this later) of a

Hermitian operator is a real quantity. This can easily be seen, for instance, in Hermitian Hamiltonian operators, where the Weyl transforms correspond to the classical expression for the energies, which are real. We also have the relation

$$\operatorname{Re} F^r(1,2) = i\varepsilon(t_1 - t_2) \operatorname{Im} F^r(1,2) \tag{31}$$

where the skew-symmetric function $\varepsilon(t_1 - t_2)$ is defined as

$$\varepsilon(t_1 - t_2) = \theta(t_1 - t_2) - \theta(t_2 - t_1) \tag{32}$$

For further simplications of Eq. (22), we define the Hermitian functions

$$A(1,2) = -2 \operatorname{Im} G^r(1,2) = i[G^>(1,2) - G^<(1,2)] \tag{33}$$

$$\Gamma(1,2) = -2 \operatorname{Im} \Sigma^r(1,2) = i[\Sigma^>(1,2) - \Sigma^<(1,2)] \tag{34}$$

which also allows us to write

$$\operatorname{Re} G^r(1,2) = \frac{-i}{2} \varepsilon(t_1 - t_2)\, A(1,2) \tag{35}$$

$$\operatorname{Re} \Sigma^r(1,2) = \frac{-i}{2} \varepsilon(t_1 - t_2)\, \Gamma(1,2) \tag{36}$$

These were also employed by Kadanoff and Baym(1) for defining real quantities from the Green's functions and self-energies. Thus, Eq. (22) can be written as

$$\frac{1}{i}[G^{0-1} - \Sigma^\delta - \operatorname{Re}\Sigma^r, G^{\gtrless}] - \frac{1}{i}[\Sigma^{\gtrless}, \operatorname{Re} G^r] = \frac{1}{2}\{\Sigma^{\gtrless}, A\}, - \frac{1}{2}\{\Gamma, G^{\gtrless}\} \tag{37}$$

which is the same as that obtained by using the analytic-continuation procedure of Kadanoff and Baym.(16)

Equation (37) is completely solved if we know $G^<$ and $G^>$. However, it is more convenient to know $G^<$ and $G^r$ or $G^>$ and $G^a$, since any one of these combinations describes both densities and the propagation of disturbances in the medium, and hence give a complete description of a nonequilibrium process. For obtaining the time evolution equation of a generalized Wigner distribution transport equation, we require the time evolution equation for $G^<$ and knowledge of $G^r$. The equation for $G^<$ is given by Eq. (37). The equation for $G^r$ can easily be obtained from Eq. (14a) by taking the difference of the appropriate equation for $G^<$ and $G^>$ contained in Eq. (14a). A more straighforward and rigorous procedure is to convert the "contour" integral in Eq. (5) into integration on the real-time axis. This is done following Schwinger,⁽³⁾ Craig,⁽¹⁸⁾ Korenman,⁽¹⁵⁾ or Keldysh⁽²⁾ to yield the same matrix equation result as follows:

$$\begin{pmatrix} 0 & (G^{0-1}-\Sigma^\delta)G^a \\ (G^{0-1}-\Sigma^\delta)G^r & (G^{0-1}-\Sigma^\delta)F \end{pmatrix} - \begin{pmatrix} 0 & \Sigma^a G^a \\ \Sigma^r G^r & \Omega G^a + \Sigma^r F \end{pmatrix} = \delta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{38}$$

where

$$F = G^> + G^<$$

$$\Omega = \Sigma^> + \Sigma^<$$

Equating the matrix elements yields the equations for $G^r$, $G^a$, and $F$ given by Keldysh.⁽²⁾ We have

$$(G^{0-1} - \Sigma^\delta)G^r = 1 + \Sigma^r G^r \tag{39}$$

$$(G^{0-1} - \Sigma^\delta)G^a = 1 + \Sigma^a G^a \tag{40}$$

$$(G^{0^{-1}} - \Sigma^\delta)F = \Omega G^a + \Sigma^r F \tag{41}$$

These are the differential forms of the equations. One can also obtain the integral forms using the Dyson equation in the time contour of Eq. (10), by converting to real-time axis integration according to Schwinger,⁽³⁾ Craig,⁽¹⁸⁾ and Keldysh⁽²⁾ and employing the linear canonical matrix transformation of Keldysh.⁽²⁾ The following matrix equation results:

$$\begin{pmatrix} 0 & G^a \\ G^r & F \end{pmatrix} = \begin{pmatrix} 0 & G^{0a} \\ G^{0r} & F^0 \end{pmatrix} + \begin{pmatrix} 0 & G^{0a}\Sigma^a G^a \\ G^{0r}\Sigma^r G^r & F^0\Sigma^a G^a + G^{0r}(\Omega G^a + \Sigma^r F) \end{pmatrix} \tag{42}$$

where the self-energies include the $\Sigma^\delta$. Equation (42) yields the integral equation for $G^r$, $G^a$, and $F$,

$$G^r = G^{0r} + G^{0r}\Sigma^r G^r \tag{43}$$

$$G^a = G^{0a} + G^{0a}\Sigma^a G^a \tag{44}$$

$$F = F^0(1 + \Sigma^a G^a) + G^{0r}(\Omega G^a + \Sigma^r F) \tag{45}$$

Using Eq. (39), or Eq. (43), as obtained from Eq. (10), with corresponding results obtained from Eq. (11), and using the notation of self-energies in Eqs. (42)–(45), we may write Eq. (45) as

$$F = (1 + G^r \Sigma^r) F^0 (1 + \Sigma^a G^a) + G^r \Omega G^a \tag{45a}$$

The integral equation for $G^<$ can now be readily obtained from the above results, since

$$G^< = \tfrac{1}{2}(F - G^r + G^a) \tag{46}$$

The same result for the integral form of $G^<$ can be obtained directly from Eq. (10) by converting the integration to the real-time axis, employing Schwinger's definition of the matrix form of the nonequilibrium Green's function on the real-time axis,(3) but without use of the Keldysh transformation,(2) to yield the following matrix relation:

$$\begin{pmatrix} G^c & -G^< \\ -G^> & \tilde{G}^c \end{pmatrix} = \begin{pmatrix} G_0^c & -G_0^< \\ -G_0^> & \tilde{G}_0^c \end{pmatrix} + \begin{pmatrix} \begin{bmatrix} G_0^c(\Sigma^c G^c - \Sigma^< G^>) \\ -G_0^<(\Sigma^> G^c - \tilde{\Sigma}^c G^>) \end{bmatrix} & \begin{bmatrix} G_0^c(\Sigma^< \tilde{G}^c - \Sigma^c G^<) \\ -G_0^<(\tilde{\Sigma}^c \tilde{G}^c - \Sigma^> G^<) \end{bmatrix} \\ \begin{bmatrix} G_0^>(\Sigma^c G^c - \Sigma^< G^>) \\ -\tilde{G}_0^c(\Sigma^> G^c - \tilde{\Sigma}^c G^>) \end{bmatrix} & \begin{bmatrix} G_0^>(\Sigma^< \tilde{G}^c - \Sigma^c G^<) \\ -\tilde{G}_0^c(\tilde{\Sigma}^c \tilde{G}^c - \Sigma^> G^<) \end{bmatrix} \end{pmatrix} \tag{47}$$

where $G^c$ $(= G^r + G^<)$ stands for the chronological Green's function and $\tilde{G}^c$ $[= -(G^a - G^<)]$ is the antichronological Green's function, with a similar definition for the self-energies. Equating the matrix elements for $G^{\gtrless}$, we have

$$G^{\gtrless} = G_0^{\gtrless}(1 + \Sigma^a G^a) + G_0^r(\Sigma^{\gtrless} G^a + \Sigma^r G^{\gtrless}) \tag{48}$$

which gives exactly the identical result for $G^<$ as that obtained from Eq. (46). We also note that adding the equations for $G^>$ and $G^<$ of (48) gives the equation for $F$ in Eq. (45), just as the sum of the differential equations for $G^<$, and $G^>$ in Eq. (14a) gives the differential equation for $F$ in Eq. (41). Separating the terms that depend explicitly on the boundary condition (i.e., initial condition), we may write Eq. (48), using Eq. (43) for $G^r$, as

$$G^{\gtrless} = G^r \Sigma^{\gtrless} G^a + (1 - G_0^r \Sigma^r)^{-1} G_0^{\gtrless}(1 + \Sigma^a G^a) \tag{49}$$

which can also be written as

$$G^{\gtrless} = G^r \Sigma^{\gtrless} G^a + (1 + G^r \Sigma^r)\, G_0^{\gtrless}(1 + \Sigma^a G^a) \tag{50}$$

where the second term in the last equation depends on the initial condition. Note that by adding the equations for $G^<$ and $G^>$ in Eq. (50) gives the equation for $F$ given by Eq. (45a).

## 3. PHASE-SPACE FREQUENCY–TIME DOMAIN EVOLUTION EQUATION OF A QUANTUM DISTRIBUTION FUNCTION

Let us rewrite the differential equation for $G^<$ in Eq. (37) as

$$\begin{aligned}\left(\frac{\partial}{\partial t_1} + \frac{\partial}{t_{1'}}\right) G^<(1, 1') = {} & \frac{1}{i\hbar}\,[\tilde{\mathscr{H}}, G^<](1, 1') \\ & + \frac{1}{i\hbar}\,[\Sigma^<, \operatorname{Re} G^r](1, 1') \\ & + \frac{1}{2\hbar}\,\{\Sigma^<, A\}(1, 1') - \frac{1}{2\hbar}\,\{\Gamma, G^<\}(1, 1')\end{aligned} \tag{51}$$

where

$$\tilde{\mathscr{H}} = \mathscr{H} + \operatorname{Re} \Sigma^r \tag{52}$$

We transform the space-time variables as follows:

$$\begin{aligned} t_1 &= T - \tau/2, & \mathbf{r}_1 &= \mathbf{q} - \mathbf{v}/2 \\ t_{1'} &= T + \tau/2, & \mathbf{r}_{1'} &= \mathbf{q} + \mathbf{v}/2 \end{aligned} \tag{53}$$

We define 4-dimensional vectors in terms of these variables and their conjugate variables following Schwinger$^{(3)}$ as

$$\begin{aligned} p &= (\mathbf{p}, E), \qquad E = \hbar\omega \\ q &= (\mathbf{q}, T) \\ v &= (\mathbf{v}, \tau) \end{aligned} \tag{54}$$

In terms of these variables, we can immediately write Eq. (51) as

$$\begin{aligned}\frac{\partial}{\partial T} G^<(\mathbf{v}, \tau, \mathbf{q}, T) = {} & \frac{1}{i\hbar}\,[\tilde{\mathscr{H}}, G^<](\mathbf{v}, \tau, \mathbf{q}, T) \\ & + \frac{1}{i\hbar}\,[\Sigma^<, \operatorname{Re} G^r](\mathbf{v}, \tau, \mathbf{q}, T) \\ & + \frac{1}{2\hbar}\,\{\Sigma^<, A\}(\mathbf{v}, \tau, \mathbf{q}, T) - \frac{1}{2\hbar}\,\{\Gamma, G^<\}(\mathbf{v}, \tau, \mathbf{q}, T)\end{aligned} \tag{55}$$

The Weyl transform $a(p, q)$ of any operator $\hat{A}$ is defined by the relation$^{(17)}$

$$a(p, q) = \int dv\ e^{(i/\hbar)\, p \cdot v} \langle q - \tfrac{1}{2}v \,|\hat{A}|\, q + \tfrac{1}{2}v \rangle$$

$$\equiv \mathscr{W} A(\mathbf{v}, \tau, \mathbf{q}, T) \tag{56}$$

Therefore, if we take the Weyl transform of both sides of Eq. (55), we obtain a phase-space frequency–time domain evolution equation for $G^{<}(p, q)$.

To evaluate the Weyl transform of the terms involving commutator and anticommutator on the right-hand side of Eq. (55), we need the following result valid for any two operators $A$ and $B$:

$$\mathscr{W}[A, B](\mathbf{v}, \tau, \mathbf{q}, T) = 2i \sin(\hat{\Lambda})\, a(p, q)\, b(p, q) \tag{57}$$

$$\mathscr{W}\{A, B\}(\mathbf{v}, \tau, \mathbf{q}, T) = 2 \cos(\hat{\Lambda})\, a(p, q)\, b(p, q) \tag{58}$$

where

$$\hat{\Lambda} = \frac{\hbar}{2} \left( \frac{\partial^{a}}{\partial q} \cdot \frac{\partial^{b}}{\partial p} - \frac{\partial^{a}}{\partial p} \cdot \frac{\partial^{b}}{\partial q} \right)$$

is the "Poisson bracket" operator. Applying these results to Eq. (55), we have the evolution equation for $G^{<}(p, q)$ given as

$$\begin{aligned}
\frac{\partial}{\partial T} G^{<}(\mathbf{p}, E, \mathbf{q}, T) = {} & \frac{2}{\hbar} \sin(\hat{\Lambda})\, \tilde{H}(p, q)\, G^{<}(p, q) \\
& + \frac{2}{\hbar} \sin(\hat{\Lambda})\, \Sigma^{<}(p, q)\, \mathrm{Re}\, G^{r}(p, q) \\
& + \frac{1}{\hbar} \cos(\hat{\Lambda})\, \Sigma^{<}(p, q)\, A(p, q) \\
& - \frac{1}{\hbar} \cos(\hat{\Lambda})\, \Gamma(p, q)\, G^{<}(p, q)
\end{aligned} \tag{59}$$

To the author's knowledge, Eq. (59) has not been given in the literature. What is usually given by most authors are the first few terms of Eq. (59), obtained from the very beginning of their formulations, corresponding to the first-order terms in the gradient expansion of Eq. (59) to derive the quantum Boltzmann equation (QBE). Indeed, it easy to see that, by writing

$$\frac{\partial G^{<}}{\partial T}(\mathbf{p}, E, \mathbf{q}, T) = -\left( \frac{\partial^{(E)}}{\partial T} \frac{\partial^{(G^{<})}}{\partial E} - \frac{\partial^{(E)}}{\partial E} \frac{\partial^{(G^{<})}}{\partial T} \right) E G^{<}(\mathbf{p}, E, \mathbf{q}, T) \tag{60}$$

expanding Eq. (59) to first order in the gradient, using Eqs. (33) and (34) for the definition of $A$ and $\Gamma$, and noting that Kadanoff and Baym define the Weyl transform with the multiplier *i*, we immediately recover the basic and classic result of QBE, given by Kadanoff and Baym [Eq. (9.30) of ref. 1]. Note that to first order in the gradient expansion, the last term of Eq. (59) resembles the relaxation-time approximation for "dilute" systems. However, all QBE results do not give the original Wigner distribution function equation in the limit of vanishing self-energies, and these clearly reflect the inadequacies of QBE for the application to a realistic simulation of quantum-based semiconductor devices. Therefore, all QBE results given in the literature are not applicable to advancing the numerical simulation of resonant-tunneling devices(7–12) to include all many-body effects and scattering mechanisms. Indeed, Eq. (59) also gives a more general result valid for particles with arbitrary energy–momentum relation, given by Kubo *et al.*(19) in the limit of vanishing self-energies or in the absence of collision terms.

For numerical simulation purposes, an exact integral form of Eq. (59) is most useful, and is the form which reduces in the limit of vanishing self-energies to the original Wigner distribution function equation, which has been successfully used in the numerical simulation of RTD.(7–10) To convert to the integral operator form from the differential operator (trigonometric function of Poisson bracket operator) in the right-hand side of Eq. (59), we need the following general results, using 4-dimensional vectors derived in Appendix A,

$$\sin(\hat{A})\, a(p,q)\, b(p,q) = \frac{1}{(h^4)^2} \int dq'\, dp'\, K_a^s(p, q-q'; q, p-p')\, b(p', q') \tag{61}$$

$$\cos(\hat{A})\, a(p,q)\, b(p,q) = \frac{1}{(h^4)^2} \int dq'\, dp'\, K_a^c(p, q-q'; q, p-p')\, b(p', q') \tag{62}$$

where

$$\begin{aligned} &K_a^s(p, q-q'; q, p-p') \\ &\quad = \int dv\, dj \exp\left[\frac{2i}{\hbar} j\cdot(q-q')\right] \\ &\qquad \times \left\{ a\left(p-j, q+\frac{v}{2}\right) - a\left(p+j, q-\frac{v}{2}\right)\right\} \sin\frac{(p-p')}{\hbar}\cdot v \end{aligned} \tag{63}$$

$$\begin{aligned} &K_a^c(p, q-q'; q, p-p') \\ &\quad = \int dv\, dj \exp\left[\frac{2i}{\hbar} j\cdot(q-q')\right] \\ &\qquad \times \left\{ a\left(p+j, q-\frac{v}{2}\right) + a\left(p-j, q+\frac{v}{2}\right)\right\} \cos\frac{(p-p')}{\hbar}\cdot v \end{aligned} \tag{64}$$

Applying the results given by Eqs. (61)–(64) in Eq. (59) and replacing $T$ by $t$, we have the exact integral operator expression of the rhs of Eq. (59) given by

$$
\begin{aligned}
\frac{\partial}{\partial t} G^{<}(\mathbf{p}, E, \mathbf{q}, t) = {} & \frac{2}{(h^4)^2} \int dq'\, dp'\, K^{s}_{\bar{H}}(p, q-q'; q, p-p')\, G^{<}(p', q') \\
& + \frac{2}{(h^4)^2} \int dq'\, dp'\, K^{s}_{\Sigma^{<}}(p, q-q'; q, p-p')\, \mathrm{Re}\, G^{r}(p', q') \\
& - \frac{2}{(h^4)^2} \int dq'\, dp'\, K^{c}_{\Sigma^{<}}(p, q-q'; q, p-p')\, \mathrm{Im}\, G^{r}(p', q') \\
& - \frac{1}{(h^4)^2} \int dq'\, dp'\, K^{c}_{\Gamma}(p, q-q'; q, p-p')\, G^{<}(p', q') \qquad (65)
\end{aligned}
$$

Equation (65) is the most general expression for the time evolution of the particle density, $-iG^{<}(\mathbf{p}, E, \mathbf{q}, t)$, in the phase-space/frequency–time domain. It describes all nonlocalities in the phase-space and energy–time domain, and therefore incorporates the "broadening" of a $\delta$-function of energy due to "intracollisional field effects," and the broadening in a $\delta$-function of the time due to memory effects, in addition to the usual nonlocalities in the phase space of any scattering process.

The time evolution of a generalized Wigner distribution function $f_w(\mathbf{p}, \mathbf{q}, t)$, which corresponds to the classical distribution function in the kinetic theory of gases, follows from Eq. (65) by multiplying both sides of the equation by $-i$ and integrating over all energies. Here we use the definition of Wigner distribution function in terms of field operators as the statistical ensemble average of the second quantized Klimontovich operator,(17)

$$
f_w(\mathbf{p}, \mathbf{q}, t) = \int d\mathbf{v}\, e^{(i/\hbar)\mathbf{p}\cdot\mathbf{v}} \left\langle \psi^{\dagger}\left(\mathbf{q} + \frac{\mathbf{v}}{2}, t\right) \psi\left(\mathbf{q} - \frac{\mathbf{v}}{2}, t\right) \right\rangle \qquad (66)
$$

Expressed in terms of Green's function, we have

$$
\begin{aligned}
f_w(\mathbf{p}, \mathbf{q}, t) &= \int d\mathbf{v}\, e^{i\mathbf{p}\cdot\mathbf{v}} - iG^{<}\left(\mathbf{q} - \frac{1}{2}\mathbf{v}, t; \mathbf{q} + \frac{1}{2}\mathbf{v}, t\right) \\
&= \frac{1}{h} \int dv\, dE\, e^{(i/\hbar)\, p\cdot v} - iG^{<}\left(q - \frac{v}{2}, q + \frac{1}{2} v\right) \\
&= \frac{1}{h} \int dE - iG^{<}(\mathbf{p}, E, \mathbf{q}, t) \qquad (67)
\end{aligned}
$$

where we have switch to the 4-dimensional vector notation in the second line of Eq. (67). Therefore Eq. (65) becomes

$$\begin{aligned}
&\frac{\partial}{\partial t} f_w(\mathbf{p}, \mathbf{q}, t)\\
&\quad = \frac{2}{(h^4)^2 h} \int dq'\, dp'\, dE\, K^s{}_{\tilde{H}}(p, q-q'; q, p-p')(-i)\, G^<(p', q')\\
&\qquad + \frac{2}{(h^4)^2 h} \int dq'\, dp'\, dE\, K^s_{\Sigma^<}(p, q-q'; q, p-p')(-i)\, \mathrm{Re}\, G^r(p', q')\\
&\qquad - \frac{2}{(h^4)^2 h} \int dq'\, dp'\, dE\, K^c_{\Sigma^<}(p, q-q'; q, p-p')(-i)\, \mathrm{Im}\, G^r(p', q')\\
&\qquad - \frac{1}{(h^4)^2 h} \int dq'\, dp'\, dE\, K^c_{\Gamma}(p, q-q'; q, p-p')(-i)\, G^<(p', q') \qquad (68)
\end{aligned}$$

Equation (68) represents an exact integral form of the equation for a Wigner distribution function in many-body quantum transport theory, which include all scattering mechanisms, all many-body effects, and all nonlocalities in the phase-space and frequency–time domain. Hence, Eqs. (65) and (68) describe all types of transport phenomena without any restriction on the variation of all quantities in phase space. The first two terms in the rhs of Eqs. (65) and (68), which derive from a commutation of two operators in Eq. (37), may be viewed as describing the motion of particles in phase space with a more complicated energy–momentum relation due to the influence of potential and scatterings. The last two terms in these equations, which derive from the anticommutation of two operators in Eq. (37), describe particle transfers in phase space due to collisions and scatterings and correspond to the collision terms in the classical Boltzmann equation. In other words, whereas the first two terms of Eqs. (65) and (68) account for the complicated quantization of particle motion (i.e., include quantum tunneling and interference phenomena) in phase space, the last two terms account for the "broadening effects" on these motions due to scatterings and collisions. Indeed, for slowly varying systems, and for conditions of the validity of QBE to hold, the contributions coming from the second terms of Eqs. (65) and (68) can also be neglected, leading to a relaxation type of approximation to the collision terms in the QBE.

## 4. EVALUATION OF THE SELF-ENERGIES

A diagrammatic evaluation of the nonequilibrium Green's function defined on a contour is analogous to its equilibrium counterpart(18),[2] and

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[2] However, see refs. 14 and 20 for exceptional cases.

therefore leads us to consider the corresponding fundamental quantities of many-body theory(21) in terms of an "effective interaction" (closely related or referred to as the scattering amplitude or vertex function) and self-energies evaluated in an analogous manner to that of equilibrium many-body theory. Effective interactions also often obey the Dyson equation with a "proper self-energy" $\pi$ represented by the proper polarization diagrams for the two-body Coulomb interactions, and by the sum of the so-called "bubble diagrams" for interactions involving the exchange of phonons.

The first-order and lowest-order "irreducible" diagrams for the self-energy are often referred to as the Hartree–Fock approximation. For electron–impurity scattering in impure systems this corresponds to the virtual-crystal approximation. These first-order diagrams will only result in the renormalization of the energy–momentum relation for the particle. Next-order self-energy diagrams for electron–electron interactions are called the Born diagrams, and are similar to the Born approximation for the lowest-order self-energy for the electron–phonon interactions.

Higher levels of approximation for the self-energies involve infinite resummation with a selected class of "irreducible diagrams" to all orders in the perturbation. Most often this approach leads to the well-known Dyson equation for the quantity being sought. The self-energy is expressed in terms of the effective interaction or vertex function, which is approximated as a summation to all orders of bubble diagrams or "ladder" diagrams, as in the random-phase approximation (RPA) or $t$-matrix approximation to the vertex function. The RPA diagrams correspond to the use of the dressed or effective interaction in the Born approximation.(22)

For electron scattering by impurities the single-site $t$-matrix method involves infinite resummation of all terms involving repeated scattering by the same impurity site or repeated multiple scattering by the same impurity. This result in a self-energy expression which can either be given linear in the impurity concentration for the low-concentration limit, as well as including all orders of the concentation for large concentration of defects, which reduces to the virtual-crystal approximation in the limit when the relative concentration of defects approaches one.(23) More accurate approximation schemes for the self-energy of electron–impurity scattering go by the name of the coherent potential approximation (CPA) and are basically obtained by summing the same single-site diagrams as before but using an "effective medium" Green's function instead of the unperturbed Green's function of the host lattice, with self-consistent scattering potential.(23)

## 4.1. Self-Energy for Scattering by Impurities

For quantum-based devices made of "decent" (low concentration of defects) semiconductor materials, an approximation to the self-energy can use the single-site $t$-matrix approach for the retarded self-energy. In order to apply to the transport equation derived in Section 3, we need to use Weyl-transform quantities. Confining ourselves to pure Coulombic interaction with the defects (i.e., excluding spin-dependent interactions and/or the "Kondo effect"), we can write the Weyl transform of the retarded(22) self-energy as

$$\Sigma^r(p, q) = n_i T(p, q) \tag{69}$$

where $n_i$ is the impurity density, and $T(p, q)$ is the Weyl transform of the $T$-matrix operator, which can be a very complicated function of the single-site $t$-matrix. Note that, in general, the multiple single-site scattering approach will result in expressions for the self-energies which have a linear dependence on the impurity density $n_i$. The Weyl transform of the $T$-matrix obeys the following equation:

$$\begin{aligned} T(p, q) = V(p, q) + \frac{1}{(h^4)^2} \int dv\, dv'\, dj\, dj'\, e^{(i/\hbar) j \cdot v'} e^{-(i/\hbar) j' \cdot v} \\ \times V\left(p + j, q - \frac{v}{2}\right) T\left(p + j', q + \frac{v'}{2}\right) \end{aligned} \tag{70}$$

where $V(p, q)$ is the Weyl transform of the impurity potential. From the identity relations (in 4-dimensional vector notation)

$$\frac{1}{h^4} \int dq\, e^{(-i/\hbar)(k-k') \cdot q} a(p, q) = a_{kk'}\, \delta\left(p - \frac{k+k'}{2}\right) \tag{71}$$

$$a(p, q) = \int d(k-k')\, e^{(i/\hbar)(k-k') \cdot q}\, a_{kk'}\, \delta\left(p - \frac{k+k'}{2}\right) \tag{72}$$

one can readily show that indeed by performing the transformation of Eq. (71) the following equation results:

$$\begin{aligned} &\frac{1}{h^4} \int dq \exp^{\times (i/\hbar)(k-k') \cdot q}\, T(p, q) \\ &\quad = \frac{1}{(h^4)^3} \int dq\, dv\, dv'\, dj\, dj' \\ &\qquad \times e^{-(/\hbar) j' \cdot v'} e^{-(i/\hbar) j' \cdot v} e^{-(i/\hbar)(k-k') \cdot q} \\ &\qquad \times V\left(p + j, q - \frac{v}{2}\right) T\left(p + j', q + \frac{v'}{2}\right) \\ &\qquad + \frac{1}{h^4} \int dq\, e^{-(i/\hbar)(k-k') \cdot q}\, V(p, q) \end{aligned} \tag{73}$$

which reduces to the equation (in 4-dimensional vector notation) in "momentum" space

$$T_{kk'} = V_{kk'} + \int d\eta \; V_{k\eta} T_{\eta k'} \tag{74}$$

The above equation can easily be shown to be identical to the integral equation for the $T$-matrix given by Mahan.(24)

So far we have only obtained "retarded quantities" through analogy with equilibrium scattering theory. However, for impurity scattering problems, the equation for the self-energy defined on the contour is mathematically similar to that of the Green's function defined on the contour, Eq. (10). Therefore, using the same procedure for converting the equation defined on the contour to an equation defined in real time, we arrive at an equation similar to Eq. (47) for the self-energy instead of the Green's function. Equating the matrix elements of $\Sigma^{\gtrless}$, we also obtain an equation similar to Eq. (50), without the second term, since $\Sigma_0^{\gtrless}$ is zero for impurity scattering. We have

$$\Sigma^{\gtrless} = \Sigma^r G^{\gtrless} \Sigma^a \tag{75}$$

which can be written in terms of Weyl transform quantities as

$$\begin{aligned} \Sigma^{\gtrless}(p, q) = \frac{1}{(h^4)^4} \int & d\eta \, d\eta' \, d\beta \, d\beta' \, dv \, dv' \, dj \, dj' \\ & \times e^{-(1/\hbar)\beta \cdot \eta'} e^{-(i/\hbar)\beta' \cdot \eta} e^{-(i/\hbar) j \cdot v'} e^{-(i/\hbar) j' \cdot v} \\ & \times \Sigma^r \left( p + \beta + j, q - \frac{\eta}{2} - \frac{v}{2} \right) \\ & \times G^{\gtrless} \left( p + \beta + j', q - \frac{\eta}{2} + \frac{v'}{2} \right) \Sigma^a \left( p + \beta', q + \frac{\eta'}{2} \right) \end{aligned} \tag{76}$$

Using Eq. (71) applied to both sides of Eq. (76), we arrive, as we should, at the following result:

$$\Sigma^{\gtrless}(k, k') = \int d\delta \, d\eta \; \Sigma^r(k, \delta) \, G^{\gtrless}(\delta, \eta) \, \Sigma^a(\eta, k') \tag{77}$$

which, with random-impurity-distribution averaging and without external potential, yields

$$\Sigma^{\gtrless}(k, k) = n_i \int d\eta \; |T_{k\eta}|^2 \, G^{\gtrless}(\eta) \tag{78}$$

where use is made here of the relation $[\Sigma^r]^\dagger = \Sigma^a$. The above result is also given by Mahan.(24) For simulating quantum-based devices the self-energies must be calculated self-consistently using Eq. (76) or Eq. (77) together with Eq. (72). From Eqs. (34) and (76), we have

$$\begin{aligned}\Gamma(p,q)=&\frac{1}{(h^4)^4}\int d\eta\, d\eta'\, d\beta\, d\beta'\, dv\, dv'\, dj\, dj'\\ &\times\exp\left[\frac{-i}{\hbar}(\beta\cdot\eta'+\beta'\cdot\eta+j\cdot v'+j'\cdot v)\right]\\ &\times\Sigma^r\left(p+\beta+j, q-\frac{\eta}{2}-\frac{v}{2}\right)A\left(p+\beta+j', q-\frac{\eta}{2}+\frac{v'}{2}\right)\\ &\times\Sigma^a\left(p+\beta', j+\frac{\eta'}{2}\right)\end{aligned}\tag{79}$$

In "momentum" space, using Eqs. (34) and (77), the above equation reduces to an equation corresponding to Eq. (74),

$$\Gamma(k,k')=\int d\delta\, d\eta\, \Sigma^r(k,\delta)\, A(\delta,\eta)\, \Sigma^a(\eta,k')\tag{80}$$

In applying to the general quantum transport equation, Eq. (68), $\Sigma^<(p,q)$ and $\Gamma(p,q)$, which determine the kernel of integration, will have to be calculated self-consistently from Eqs. (76) and (79), respectively. The numerical implementation for doing the simulation will involve an iterative scheme to incorporate the necessary self-consistency, discussed in Section 5.

## 4.2. Electron Scattering with Quantized "Boson" Wave Field

The scattering of particles in a solid by a quantized "boson" wave field is generally described by a second-quantized Hamiltonian operator having the general from$^{(25-27)}$

$$H=H_P(\Psi^\dagger,\Psi)+H_F(\pi,\phi)+H_{PF}(\Psi^\dagger,\Psi.\pi,\phi)\tag{81}$$

where

$$H_P(\Psi^\dagger,\Psi)=\sum_{\mathbf{R},\alpha}\Psi^\dagger_\alpha(\mathbf{R},t)\,E_\alpha\left(-\frac{\hbar}{i}\nabla_{\mathbf{R}}\right)\Psi_\alpha(\mathbf{R},t)\tag{82}$$

$$H_F(\pi,\phi)=\sum_{\mathbf{R}}\left[\frac{\pi^2(\mathbf{R},t)}{2\gamma}+\begin{cases}\frac{1}{2}g|\nabla A|^2], & \text{em field}\\ \frac{1}{2}|\nabla_{\mathbf{R}}P(\mathbf{R},t)|^2], & \text{acoustic phonons}\\ \frac{1}{2}\omega^2P^2(\mathbf{R},t)], & \text{polar crystal}\end{cases}\right.\tag{83}$$

$$H_{PF}(\Psi_1^\dagger,\Psi,\pi,\phi)=-\sum_{\mathbf{R},\alpha,\beta}\Psi^\dagger_\alpha(\mathbf{R},t)\,\gamma^i_{\alpha\beta}(\mathbf{R})\,\Psi_\beta(\mathbf{R},t)\begin{cases}P_i(\mathbf{R},t), & \text{phonons}\\ A_i(\mathbf{R},t), & \text{photons}\end{cases}\tag{84}$$

$E_\alpha(k)$ is the energy-band function of Bloch electrons, $\mathbf{R}$ denotes the lattice point coordinate,$^{(17)}$ and the summation convention for all indices is used. For phonons in a solid, the scalar $\gamma$ is related to the ratio of atomic mass to the effective charge of resulting dipole moments and $g$ is related to the elastic constant of a lattice of atoms. The Greek indices include all quantum labels. For an electromagnetic wave field, $\gamma = 1/4\pi c^2$ and $g = 1/4\pi$. The equal-time commutation rules for the field operators are as follows:

A. For matter-wave field operators:

$$\{\Psi^\dagger_\alpha(\mathbf{R}, t), \Psi^\dagger_\beta(\mathbf{R}', t)\} = \{\Psi_\alpha(\mathbf{R}, t), \Psi_\beta(\mathbf{R}', t)\} = 0 \tag{85}$$

$$\{\Psi_\alpha(\mathbf{R}, t), \Psi^\dagger_\beta(\mathbf{R}', t)\} = \delta_{\alpha\beta}\delta_{\mathbf{RR}'} \tag{86}$$

B. For the phonon wave field ($\phi \equiv P$):

$$[\pi_l(\mathbf{R}, t), P_j(\mathbf{R}', t)] = \frac{\hbar}{i}\delta_{lj}\,\delta_{\mathbf{RR}'} \tag{87}$$

$$[\pi_l(\mathbf{R}, t), \pi_j(\mathbf{R}', t)] = [P_l(\mathbf{R}, t), P_j(\mathbf{R}', t)] = 0 \tag{88}$$

C. For the electromagnetic photon wave field ($\pi_l = \dot{A}_l/4\pi c^2$):

$$[A_l(\mathbf{R}, t), A_j(\mathbf{R}', t)] = [\pi_l(\mathbf{R}, t), \pi_j(\mathbf{R}, t)] = 0 \tag{89}$$

$$[\pi_l(\mathbf{R}, t), A_j(\mathbf{R}', t)] = \frac{\hbar}{i}\delta^T_{lj}\delta^T_{\mathbf{RR}'} \tag{90}$$

where $\delta^T_{lj}\,\delta^T_{\mathbf{RR}'}$ is the so-called transverse $\delta$-function ($\nabla \cdot \mathbf{A} = 0$), which in the continuum limit is given by

$$\delta^T_{lj}(\mathbf{x} - \mathbf{x}') = \frac{1}{(h)^3}\int d\mathbf{k}^3 \left\{\exp\left[\frac{i\mathbf{k}}{\hbar}\cdot(\mathbf{x} - \mathbf{x}')\right]\right\}\left(\delta_{lj} - \frac{k_l k_j}{k^2}\right) \tag{91}$$

Note the universal form of the interaction Hamiltonian operator given by Eq. (84), characterizing the interaction of the quantized wave field with the particles. Indeed, the impurity scattering interaction Hamiltonian operator discussed in the previous section can also be cast in the form of Eq. (84) (e.g., the Hamiltonian of the famous Kondo problem in dilute magnetic alloys).

The coupling matrix $\gamma^i_{\alpha\beta}(\mathbf{R})$ in Eq. (84) has the following expressions for electrons in a solid.

A. For phonons:

$$\gamma_{\alpha\beta}(\mathbf{R}) = \int W^*_\alpha(\mathbf{x} - \mathbf{R})\left(\nabla_\mathbf{R}\frac{1}{|\mathbf{x} - \mathbf{R}|}\right)W_\beta(\mathbf{x} - \mathbf{R})\,d\mathbf{x}^3 \tag{92}$$

B. For photons:

$$\gamma_{\alpha\beta}(\mathbf{R}) = \frac{e}{mc} \int W_\alpha^*(\mathbf{x}-\mathbf{R}) \left( \frac{-\hbar}{i} \nabla_{\mathbf{x}} \right) W_\beta(\mathbf{x}-\mathbf{R})\, d\mathbf{x}^3 \tag{93}$$

C. For electron–impurity scattering (given here for completeness)

$$\gamma_{\alpha\beta}(\mathbf{R}) = \int W_\alpha^*(\mathbf{x}-\mathbf{R}) \left( \frac{Z'e^2}{|\mathbf{x}-\mathbf{R}|} e^{-\sigma \cdot (\mathbf{x}-\mathbf{R})} \right) \mathbf{S}_{\alpha\beta} W_\beta(\mathbf{x}-\mathbf{R})\, d\mathbf{x}^3 \tag{94}$$

where the $W$ function is the localized Wannier function and $\mathbf{S}_{\alpha\beta}$ is the Pauli matrix for the case of magnetic impurities.

In what follows, we will evaluate the sums over lattice points as an integral (i.e., continuum approximation of the lattice coordinates, $\sum_{\mathbf{R}} \rightarrow \int d^3\mathbf{R}$). Dropping the Greek indices, for simplicity (i.e., one-band model and spin-independent interactions), it is easy to see that the approximation to the electron self-energy for electron–phonon scattering is very similar to that which arises for the electron–electron Coulomb interaction. To see this, one writes the effective equation for the electron field operator as$^{(25)}$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Psi(x) = {} & E_\alpha \left( -\frac{\hbar}{i} \nabla_{\mathbf{x}} \right) \Psi(x) \\ & + \gamma^2 \int dx_2\, D_0(x, x_2)\, \Psi^\dagger(x_2)\, \Psi(x_2)\, \Psi(x) \\ & + \frac{1}{2} \int dx_2\, V(x, x_2)\, \Psi^\dagger(x_2)\, \Psi(x_2)\, \Psi(x) \end{aligned} \tag{95}$$

where the last term represents the electron–electron Coulomb interaction corresponding to the residual screened Coulomb interaction between Bloch electrons. The photon propagator $D_0(x_1, x_2)$ multiplied by the square of the coupling constant $\gamma$ represents the interactions between Bloch electrons through the exchange of phonons. Thus, the perturbation treatment of electron–phonon scattering is formally similar to that for the electron–electron interaction problems.$^{(22)}$

A meaningful and significant contribution to the electron–phonon self-energy is given by a "one-phonon" diagram similar to the Hartree–Fock exchange diagram of the electron–electron scattering [note that in contrast to $V(x, x_2)$, $D_0(x, x_2)$ is nonlocal in time] defined on the time contour as

$$\Sigma(1, 2) = iG(1, 2)\, D(1, 2) \tag{96}$$

Therefore by fixing the time order, we immediately obtain, in real time,

$$\Sigma^{\gtrless}(1,2) = iG^{\gtrless}(1,2)\, D^{\gtrless}(1,2) \tag{97}$$

Equation (97) immediately leads to the expression for the retarded and advanced self-energies in terms of the Green's function and phonon propagator:

$$\Sigma^{r,a}(1,2) = i[G^{r,a}(1,2)\, D^{>}(1,2) + G^{<}(1,2)\, D^{r,a}(1,2)] \tag{98}$$

To avoid the immense complication of solving the complete quantum transport equation for phonons to obtain the nonequilibrium phonon propagator, we make some simplifications. We assume that we can use the phonon propagator for a phonon system at equilibrium. Note, however, that the phonon relaxation times may be comparable to the electron transit time across the quantum region of a device.[(7-9)]

In applying the above results for phonon scattering to Eq. (68), we are interested in the Weyl transform equivalent of Eq. (97). We have, in four-dimensional vectors, Eq. (54), the following

$$\begin{aligned} \Sigma^{\gtrless}(p,q) = i \int dv\, e^{(i/\hbar)p\cdot v} & \\ &\times G^{\gtrless}(q - \tfrac{1}{2}v, q + \tfrac{1}{2}v) \\ &\times D^{\gtrless}(q - \tfrac{1}{2}v, q + \tfrac{1}{2}v) \end{aligned} \tag{99}$$

The phonon propagator for a phonon system at equilibrium satisfies

$$D^{\gtrless}(q - \tfrac{1}{2}v, q + \tfrac{1}{2}v) = D^{\gtrless}(v)$$

$$D^{\gtrless}(v) = \frac{1}{h^4}\int dk\, e^{(i/\hbar)k\cdot v}\, D^{\gtrless}(k)$$

Hence we have

$$\begin{aligned} \Sigma^{\gtrless}(p,q) &= \frac{i}{h^4}\int dk\, dv\, e^{(i/\hbar)(p+k)\cdot v} \\ &\qquad \times G^{\gtrless}(q - \tfrac{1}{2}v, q + \tfrac{1}{2}v)\, D^{\gtrless}(k) \\ &= \frac{i}{h^4}\int dk\, G^{\gtrless}(p+k, q)\, D^{\gtrless}(k) \end{aligned} \tag{100}$$

and therefore we also have

$$\begin{aligned} \Gamma(p,q) = -\frac{1}{h^4}\int dk\, \{ & G^{>}(p+k,q)\, D^{>}(k) \\ & - G^{<}(p+k,q)\, D^{<}(k)\} \end{aligned} \tag{101}$$

The expressions for the Fourier-transformed equilibrium phonon propagators are

$$D^{<}(\mathbf{k}, E') = -i\gamma_{\mathbf{k}}^2\{(N_{\mathbf{k}}+1)h\,\delta(E'+\Omega_{\mathbf{k}}) + N_{\mathbf{k}}h\,\delta(E'+\Omega_{\mathbf{k}})\} \quad (102)$$

$$D^{>}(\mathbf{k}, E') = -i\gamma_{\mathbf{k}}^2\{(N_{\mathbf{k}}+1)h\,\delta(E'+\Omega_{\mathbf{k}}) + N_{\mathbf{k}}h\,\delta(E'-\Omega_{\mathbf{k}})\} \quad (103)$$

where $\Omega_{\mathbf{k}}$ is the energy–momentum relation for phonons. Substituting the explicit expressions for $D^{>}(\mathbf{k}, E')$ and $D^{<}(\mathbf{k}, E')$ in the expression for $\Sigma^{\gtrless}(p, q)$, and $\Gamma(p, q)$ above and integrating with respect to $E'$, we obtain the following expressions:

$$\Sigma^{<}(p, q) = \frac{1}{h^3}\int d\mathbf{k}\,\{G^{<}(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}, q)\,\gamma_{\mathbf{k}}^2(N_{\mathbf{k}}+1) + G^{<}(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}, q)\,\gamma_{\mathbf{k}}^2 N_{\mathbf{k}}\} \quad (104)$$

$$\Sigma^{>}(p, q) = \frac{1}{h^3}\int d\mathbf{k}\,\{G^{>}(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}, q)\,\lambda_{\mathbf{k}}^2(N_{\mathbf{k}}+1) + G^{>}(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}, q)\,\gamma_{\mathbf{k}}^2 N_{\mathbf{k}}\} \quad (105)$$

$$\Gamma(p, q) = \frac{1}{h^3}\int d\mathbf{k}\,\{\gamma_{\mathbf{k}}^2 N_{\mathbf{k}}[A(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}, q) + A(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}, q)] + i\gamma_{\mathbf{k}}^2[G^{>}(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}, q) - G^{<}(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}, q)]\} \quad (106)$$

We note that for a uniform system at steady-state conditions (independent of $q$), the expressions for $\Sigma^{<}(p, q)$, $\Sigma^{<}(p, q)$ and $\Gamma(p, q)$ reduce to those given by Mahan.(24) For $\Gamma(p, q)$ of a uniform system at steady state, use can be made of the following exact relations:

$$-iG^{<}(\mathbf{p}, E) = f_w(\mathbf{p}, E)\,A(\mathbf{p}, \mathbf{E}) \quad (107)$$

$$iG^{>}(\mathbf{p}, \mathbf{E}) = [1 - f_w(\mathbf{p}, \mathbf{E})]\,A(\mathbf{p}, \mathbf{E}) \quad (108)$$

where

$$\frac{1}{h}\int dE\,A(\mathbf{p}, E) = 1$$

which follow from the equal-time commutation relations for the field operators. These relations are exact, since the Weyl transform of the product of operators for uniform systems at steady state reduces to the product of their Weyl transforms. However, for nonuniform system and/or the nonstationary state, this relations do not hold and the so-called "Kadanoff–Baym *Ansatz*(1,6,28)" is generally not valid for nonequilibrium transport. The "Kadanoff–Baym *Ansatz*" is only valid up to the first order in the gradient (*i.e.*, has zero-order accuracy) and the so-called "generalized Kadanoff–Baym *Ansatz*" given by Lipavský *et al.*(28) can be shown to be only valid up to the second order in the gradient expansion (Appendix B). When the last two relations are substituted in the expressions for $\Sigma^{<}(p, q)$ and $\Gamma(p, q)$, we obtain

$$\Sigma^{<}(p, q) = \frac{i}{h^3} \int d\mathbf{k} \, \{ f_w(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}) \, A(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}) \, \gamma_{\mathbf{k}}^2 (N_{\mathbf{k}}+1) + f_w(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}) \, A(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}) \, \gamma_{\mathbf{k}}^2 N_{\mathbf{k}} \} \tag{109}$$

$$\Gamma(p, q) = \frac{i}{h^3} \int d\mathbf{k} \, \{ \gamma_{\mathbf{k}}^2 [N_{\mathbf{k}} + f_w(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}})] \, A(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}) + \gamma_{\mathbf{k}}^2 [N_{\mathbf{k}} + 1 - f_w(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}})] \, A(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}}) \} \tag{110}$$

which agrees with the result given by Mahan.(24) For application to the simulation of high-speed devices using Eq. (65) or (68), the more general results will have to be used self-consistently through an iterative numerical procedure. In the next section we will use the last two equations to highlight the collision terms in Eqs. (65) and (68).

## 5. SELF-CONSISTENT SOLUTION AND SIMPLIFICATIONS OF MANY-BODY QUANTUM TRANSPORT EQUATIONS

The exact quantum transport equations (65) and (68) do not stand alone for two reasons: (a) these equations are coupled to the equation for $G^r$ (or $G^{>}$) and to "boson" field propagators, (b) the kernel of the integral operators depends on $G^r$ (or $G^{>}$) and the sought after solution $G^{<}$ (and hence $f_w$), as well as, in general, to the "boson" field propagators. In Section 4.1, we made the assumption that the phonon propagator is known and corresponds to the propagator for a phonon system at equilibrium. Besides the approximations made in the self-energy expressions, this constitutes one major simplifications of Eqs. (65) and (68), by giving up self-consistency with respect to the phonon (or interacting "boson") systems.

However, self-consistency with respect to the particle system must be retained. Following the well-known standard technique of all many-body calculations, one tries to achieve self-consistency by an iterative procedure. Therefore, in solving Eqs. (65) and (68), one uses "noninteracting" $G_0^{<}$ and $G_0^r$ (or $G_0^{>}$) to evaluate the kernel of the integral operator, and all other terms in the right-hand side (rhs) of these equations [note that $\tilde{H}(p, q)$ includes Re $\Sigma^r(p, q)$]. Then the known "operators" in the rhs of Eqs. (65)

and (68) are used to solve for new $G^<$ and $f_w$. The equation for $G^r$, Eq. (39) or (43), will also be solved for new $G^r$, after which the process may be repeated with the new set of approximate $G^<$ and $G^r$.

In the practical numerical simulation of quantum-based devices,(7–12) the first iteration of the above-mentioned self-consistency procedure may represent a more accurate enough solution, depending on the choice of the starting solutions for the iteration process. A clear choice for quantum-based device analysis would be the solutions obtained for noninteracting particles. This means that the zero-order approximation neglects all the terms except the first term in the rhs of Eqs. (65) and (68). The numerical procedure and technique for obtaining time-dependent and steady-state solutions for a resonant-tunneling device (RTD), within the effective-mass approximation for noninteracting particles, has now been established, and obtaining the solution of these devices is by now a routine task.(7–9)

When $\tilde{H}(p, q)$ in Eq. (59) can be written in the effective-mass approximation as

$$\tilde{H}(p, q) = \frac{\mathbf{p}^2}{2m^*} + V(\mathbf{q}) \tag{111}$$

where $V(\mathbf{q})$ is the potential in the device region, then Eqs. (65) and (68), in the absence of collisions and scattering, reduce to the following expressions:

$$\begin{aligned}\frac{\partial}{\partial t} G^<(\mathbf{p}, E, \mathbf{q}, t) = &-\frac{\mathbf{p}}{m^*} \nabla_{\mathbf{q}} G^<(\mathbf{p}, E, \mathbf{q}, t) \\ &+ \frac{1}{h^4} \int d\mathbf{p}'\, d\mathbf{v} \left[ V\left(\mathbf{q} + \frac{\mathbf{v}}{2}\right) - V\left(\mathbf{q} - \frac{\mathbf{v}}{2}\right) \right] \\ &\times \sin\left[ \left( \frac{\mathbf{p} - \mathbf{p}'}{\hbar} \right) \cdot \mathbf{v} \right] G^<(\mathbf{p}', E, \mathbf{q}, t)\end{aligned} \tag{65a}$$

$$\begin{aligned}\frac{\partial}{\partial t} f_w(\mathbf{p}, \mathbf{q}, t) = &-\frac{\mathbf{p}}{m^*} \nabla_{\mathbf{q}} f_w(\mathbf{p}, \mathbf{q}, t) \\ &+ \frac{1}{h^4} \int d\mathbf{p}'\, d\mathbf{v} \left[ V\left(\mathbf{q} + \frac{\mathbf{v}}{2}\right) - V\left(\mathbf{q} - \frac{\mathbf{v}}{2}\right) \right] \\ &\times \sin\left[ \left( \frac{\mathbf{p} - \mathbf{p}'}{\hbar} \right) \cdot \mathbf{v} \right] f_w(\mathbf{p}', \mathbf{q}, t)\end{aligned} \tag{68a}$$

Equations (65a) and (68a) are the well-known forms of the time evolution equation for the Wigner distribution function for noninteracting particles.

The time-dependent and steady-state solutions of these equations have been given by Frensley(7) and by Jensen and Buot.(8–9) A random-phase approximation to the electron–electron interactions within the effective-mass approximation can easily be incorporated in their numerical solutions by simultaneously solving the Poisson equation together with Eq. (68a), thus obtaining an improved initial starting value for $G_0^<$ and $G_0^r$.

Another approach, which is only of academic interest here, often taken in the literature is to obtain the time evolution equation of the Green's function to first order in the gradients, leading to the so-called quantum Boltzmann equation (QBE). Therefore, results often given in the literature correspond to the result obtained by expanding Eq. (59) up to the first order in the gradient. We immediately obtain, up to first order in the gradient expansion of Eq. (59), the following:

$$\frac{\partial G^<}{\partial t}(\mathbf{p}, E, \mathbf{q}, t) = [\tilde{H}(p,q), G^<(p,q)] + [\Sigma^<(p,q), \operatorname{Re} G^r(p,q)] + i\{\Sigma^<(p,q)\, G^>(p,q) - \Sigma^>(p,q)\, G^<(p,q)\} \tag{112}$$

where we have used the definitions of $A(p,q)$ and $\Gamma(p,q)$ from Eqs. (33) and (34), and the Poisson bracket notation of Kadanoff and Baym.(1) From the definition of $\tilde{H}(p,q)$ given by Eq. (52), and noting that Kadanoff and Baym define the Weyl transform with multiplier $i$, we immediately recognize that the last equation is identical to the one given by Kadanoff and Baym,(1) which has become the basis for almost all investigations concerning high-field transport of submicron devices.(4–6)

Clearly, the QBE result is markedly different from Eq. (65a) in the limit of vanishing self-energies and hence precludes at the outset quantum effects due to tunneling and quantum interference, and therefore is not of any use for the numerical simulation of RTD. A most instructive way to see this is to examine the effective potential as seen by the particles in Eq. (68a) compared with that of Eq. (112). Whereas in Eq. (112) the particles essentially "feel" the classical potential, plus many-body corrections from the self-energies, the particles in Eq. (65a) see an effective potential $V_{\text{eff}}$ which is the sum of a classical potential and a quantum potential, defined by the following equation(9):

$$(\nabla_{\mathbf{q}} V_{\text{eff}})\, \nabla_{\mathbf{p}} f_w(\mathbf{p}, \mathbf{q}) = \frac{1}{\hbar} \int d\mathbf{p}'\, V(\mathbf{q}, \mathbf{p} - \mathbf{p}')\, f_w(\mathbf{p}', \mathbf{q}) \tag{113}$$

where $V(\mathbf{q}, \mathbf{p})$ is defined by (68a) and may include all many-body corrections just as in Eq. (112). $V_{\text{eff}}$ is responsible for the tunneling mechanism in RTD.(9)

At the end of Section 3, we referred to the first two terms on the rhs of Eqs. (65) and (68) as describing the complicated quantization of particle motion in phase space, including quantum tunneling and interference phenomena. The first term clearly represents the motion of particles with an "effective single-particle Hamiltonian" given by Eq. (52). The second term represents "*bona fide*" many-body effects in the single-particle kinetics and may be viewed as a "second-order" kinetic correction to the particle motion due to collisions and scatterings.(14) The last two terms account for the transfer of particles in 4-dimensional vector phase space due to collisions and scatterings. To see this, let us evaluate the last two terms for a uniform system at steady-state conditions for impurity scatterings and phonon scatterings.

### 5.1. Impurity Scattering

For a uniform system at steady state, the last two terms of Eq. (65) or Eq. (59) yield

$$\begin{aligned} &\Sigma^{<}(p)\,A(p) - \Gamma(p)\,G^{<}(p) \\ &\quad = \sum_{\mathbf{k}} [W_{\mathbf{p}\leftarrow\mathbf{k}}(E)\,G^{<}(\mathbf{k}, E) - W_{\mathbf{k}\leftarrow\mathbf{p}}(E)\,G^{<}(\mathbf{p}, E)] \end{aligned} \tag{114}$$

where

$$W_{\mathbf{k}\leftarrow\mathbf{p}} = n_i |T_{\mathbf{kp}}(E)|^2\, A(\mathbf{k}, E) \tag{115}$$

$$W_{\mathbf{p}\leftarrow\mathbf{k}} = n_i |T_{\mathbf{pk}}(E)|^2\, A(\mathbf{p}, E) \tag{116}$$

Clearly the rhs of Eq. (114) is identical to the usual form of the collision operator of the Boltzmann equation.

### 5.2. Electron–Phonon Scattering

Using Eqs. (109) and (110) for obtaining $\Sigma^{<}(p)$ and $\Gamma(p)$, respectively, we can write

$$\begin{aligned} &-i[\Sigma^{<}(p)\,A(p) - \Gamma(p)\,G^{<}(p)] \\ &\quad = \sum_{\mathbf{k}} [W^{e}_{\mathbf{pk}} f_w(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}}) + W^{a}_{\mathbf{pk}} f_w(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}})] \\ &\qquad - \sum_{\mathbf{k}} [\tilde{W}^{e}_{\mathbf{pk}} f_w(\mathbf{p}, E) + \tilde{W}^{a}_{\mathbf{pk}} f_w(\mathbf{p}, E)] \end{aligned} \tag{117}$$

where

$$W^e_{\mathbf{pk}} = A(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}})\, A(\mathbf{p}, E)\, \gamma^2_{\mathbf{k}}(N_{\mathbf{k}}+1) \tag{118}$$

$$W^a_{\mathbf{pk}} = A(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}})\, A(\mathbf{p}, E)\, \gamma^2_{\mathbf{k}} N_{\mathbf{k}} \tag{119}$$

$$\tilde{W}^e_{\mathbf{kp}} = A(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}})\, A(\mathbf{p}, E)\, \gamma^2_{\mathbf{k}}[N_{\mathbf{k}}+1-f(\mathbf{p}+\mathbf{k}, E-\Omega_{\mathbf{k}})] \tag{120}$$

$$\tilde{W}^a_{\mathbf{kp}} = A(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}})\, A(\mathbf{p}, E)\, \gamma^2_{\mathbf{k}}[N_k+f(\mathbf{p}+\mathbf{k}, E+\Omega_{\mathbf{k}})] \tag{121}$$

A more revealing from for Eq. (117) is obtained if the spectral function $A(\mathbf{p}, E)$ is approximated as a delta function, $A(\mathbf{p}, E) = h\,\delta(E-E_{\mathbf{p}})$. Then Eq. (117) reduces to the form of the collision operator of a Boltzmann equation as

$$\frac{-i}{h}\int dE\,[\Sigma^<(p)\,A(p) - \Gamma(p)\,G^<(p)] = \sum_{\mathbf{k}'}[W_{\mathbf{k}\leftarrow\mathbf{k}'} f_w(\mathbf{k}') - W_{\mathbf{k}'\leftarrow\mathbf{k}} f_w(\mathbf{k})] \tag{122}$$

where

$$\begin{aligned} W_{\mathbf{k}\leftarrow\mathbf{k}'} = {} & (h)\,\delta(E_{\mathbf{k}} - E_{\mathbf{k}'} + \Omega_{\mathbf{k}'-\mathbf{k}})\,\gamma^2_{\mathbf{k}'-\mathbf{k}}(N_{\mathbf{k}'-\mathbf{k}}+1)[1-f_w(\mathbf{k})] \\ & + (h)\,\delta(E_{\mathbf{k}} - E_{\mathbf{k}'} - \Omega_{\mathbf{k}'-\mathbf{k}})\,\gamma^2_{\mathbf{k}'-\mathbf{k}} N_{\mathbf{k}'-\mathbf{k}}[1-f_w(\mathbf{k})] \end{aligned} \tag{123}$$

$$\begin{aligned} W_{\mathbf{k}'\leftarrow\mathbf{k}} = {} & (h)\,\delta(E_{\mathbf{k}} - E_{\mathbf{k}'} - \Omega_{\mathbf{k}'-\mathbf{k}})\,\gamma^2_{\mathbf{k}'-\mathbf{k}}(N_{\mathbf{k}'-\mathbf{k}}+1)[1-f_w(\mathbf{k}')] \\ & + (h)\,\delta(E_{\mathbf{k}} - E_{\mathbf{k}'} + \Omega_{\mathbf{k}'-\mathbf{k}})\,\gamma^2_{\mathbf{k}'-\mathbf{k}} N_{\mathbf{k}'-\mathbf{k}}[1-f_w(\mathbf{k}')] \end{aligned} \tag{124}$$

The last result for the collision operator agrees with the collision operator recently derived by Lin and Chiu(29) insofar as one can replace the spectral function by a delta function, as can be shown by rearrangement of terms, appropriate change of variable $\mathbf{k}'-\mathbf{k}$ to the phonon wavevector $\mathbf{q}$, and performing the sum over $\mathbf{q}$ in place of $\mathbf{k}'$. However, contrary to the claim made by them, the above forms are only valid for uniform systems at steady state. Moreover, their formalism is based on a first-order gradient expansion from the beginning and hence has very limited application to the simulation of realistic high-speed devices, characteristics of all QBE results.

For phonon scattering at low enough temperature, we may ignore the contribution of Eqs. (123), so that the contribution to the collision operator will solely come from $-\Gamma(p)\,G^<(p)$ and the rhs of Eq. (122) may be written as $-f_w(\mathbf{k})/\tau$, where $\tau$ is the relaxation time. Another approximation to Eq. (122) in terms of the relaxation-time approximation, which is strictly valid only near equilibrium, is based on the use of the normalized equilibrium distribution function $f_0(\mathbf{k})$ and proceeds as follows:

$$\sum_{\mathbf{k}'}[W_{\mathbf{k}\leftarrow\mathbf{k}'} f_w(\mathbf{k}') - W_{\mathbf{k}'\leftarrow\mathbf{k}} f_w(\mathbf{k})] = \frac{1}{\tau}\sum_{\mathbf{k}'}[f_0(\mathbf{k})\,f_w(\mathbf{k}') - f_0(\mathbf{k}')\,f_w(\mathbf{k})] \tag{125}$$

where

$$\frac{1}{\tau} = \sum_{\mathbf{k}'} W_{\mathbf{k}' \leftarrow \mathbf{k}} \tag{126}$$

$$\frac{1}{\tau} f_0(\mathbf{k}) = \langle W_{\mathbf{k} \leftarrow \mathbf{k}'} \rangle, \qquad \frac{1}{\tau} f_0(\mathbf{k}') = \langle W_{\mathbf{k}' \leftarrow \mathbf{k}} \rangle \tag{127}$$

Therefore, for constant relaxation time $\tau$, $f_0(\mathbf{k})/\tau$ represents the transition rate $W_{\mathbf{k} \leftarrow \mathbf{k}'}$ in momentum space. Recently, Frensley(12) has employed this approximation to investigate the effects of collisions on the device characteristics of RTD. This paper serves to clarify his approximation, which was guided by making an analogy to the Boltzmann equation. Since $f_w(p, q)$ is a strong function of $q$ in RTD, even at steady state,(7,9) and furthermore since $f_w(p, q)$ is far from thermal equilibrium, where complete detailed balance holds, this approximation is a poor approximation and is far from being self-consistent. The "Fokker–Planck collision operator" in $k$ space also employed by Frensley(12) does not seem to have any theoretical basis within the many-body quantum transport theory, since all derivatives are governed by the Poisson bracket operator. Moreover, for transient simulation of RTD all of the above approximations are clearly suspect. Serious numerical work is urgently needed for more accurate treatment of scattering and collisions in quantum transport.

## 6. CONCLUSIONS

We have presented a well-rounded and exact formalism of many-body quantum transport which serves to unify various approaches based on (a) the generalized quantum Boltzmann equation, (b) the time evolution equation of the Wigner distribution function first derived by Wigner, (c) density-matrix projection operator techniques, and (d) path integral techniques.(21) An elegant treatment for problems of Bloch electrons in the presence of a uniform external electromagnetic field(24) is straightforward and follows the Weyl–Wigner quantum mechanical techniques employed by the author in previous works.(30) This paper serves to fill the need of device physicists for advancing the numerical simulation of quantum-based devices, particularly tunneling devices such as RTD, to include scatterings and collisions while retaining full quantum effects such as tunneling and quantum interference. Indeed, this investigation is in part motivated by the absence in the literature of a quantum transport formulation to all orders in the gradients, suitable for realistic device analysis. The often treated generalized QBE essentially proceeds as a first-order gradient expansion from the very beginning and therefore has very limited use for modeling realistic devices. We have shed light on approximations that have been recently attempted in the literature for including scatterings in the Wigner distribution-function formulation of quantum transport for simulating quantum-based devices. Further serious and large-scale numerical work is clearly needed for more accurate understanding of the effects of scattering and collision in quantum-based electronic devices.

## APPENDIX A. EXACT INTEGRAL OPERATOR OF THE QUANTUM TRANSPORT EQUATION

Let us denote the Weyl transform of two operators $\hat{A}$ and $\hat{B}$ as $a(p, q)$ and $b(p, q)$, respectively. The Weyl transform of $\hat{A}\hat{B} = \hat{C}$ is denoted as $c(p, q)$. Then we have the relation

$$c(p, q) = [\exp(i\hat{\Lambda})]\, a(p, q)\, b(p, q) \tag{A1}$$

where $\hat{\Lambda}$ is the "Poisson bracket" operator used in the text. First let us evaluate the expression

$$\left[\exp\left(-i\frac{\hbar}{2}\frac{\partial^{(a)}}{\partial p}\cdot\frac{\partial^{(b)}}{\partial q}\right)\right] a(p, q)\, b(p, q)$$

We do this by first writing the Weyl transforms $a(p, q)$ and $b(p, q)$ as Fourier-transformed quantities:

$$a(p, q) = \int dv\, e^{(i/\hbar)p\cdot v}\, K^{a}(q - \tfrac{1}{2}v, q + \tfrac{1}{2}v) \tag{A2}$$

$$b(p, q) = \int du\, e^{(i/\hbar)q\cdot u}\, K^{b}(p + \tfrac{1}{2}u, p - \tfrac{1}{2}u) \tag{A3}$$

Making use of well-known "differential displacement" operation, we thus obtain

$$\begin{aligned}&\left[\exp\left(-i\frac{\hbar}{2}\frac{\partial^{(a)}}{\partial p}\cdot\frac{\partial^{(b)}}{\partial q}\right)\right] a(p, q)\, b(p, q)\\ &\quad = \frac{1}{h^4}\int du\, dq' \left\{\exp\left[\frac{i}{\hbar}(q - q')\cdot u\right]\right\} a\left(p + \frac{u}{2}, q\right) b(p, q')\end{aligned} \tag{A4}$$

where the inverse Fourier transform relations corresponding to Eqs. (A2)–(A3) were used to bring back Weyl-transformed quantities in Eq. (A4).

Let us write $b(p, q')$ in Eq. (A4) by making use of the alternate expression of Eq. (A3) as

$$b(p, q') = \int dv\, e^{(i/\hbar)p\cdot v}\, K^{b}(q' - \tfrac{1}{2}v, q' + \tfrac{1}{2}v) \tag{A5}$$

Applying the remaining differential operation in the Poisson bracket occurring in the exponent $\hat{\Lambda}$, proceeding in a similar manner as before, and then making a change of variables

$$\begin{aligned} \frac{u}{2} &= j \\ q - q' &= -\frac{v'}{2} \qquad \text{(A6)} \\ p - p' &= -j' \end{aligned}$$

we obtain

$$\begin{aligned} [\exp(i\hat{\Lambda})]\, a(p, q)\, b(p, q) = \frac{1}{(h^4)^2} \int dv\, dv'\, dj\, dj' \\ \times \exp\left(-\frac{i}{\hbar} j \cdot v'\right) \exp\left(-\frac{i}{\hbar} j' \cdot v\right) \\ \times a\left(p + j, q - \frac{v}{2}\right) b\left(p + j', q + \frac{v'}{2}\right) \qquad \text{(A7)} \end{aligned}$$

By a similar procedure, we have

$$\begin{aligned} &[\exp(-i\hat{\Lambda})]\, a(p, q)\, b(p, q) \\ &\quad = \frac{1}{(h^4)^2} \int dv\, dv'\, dj\, dj' \exp\left(-\frac{i}{\hbar} j \cdot v'\right) \exp\left(-\frac{i}{\hbar} j' \cdot v\right) \\ &\quad \times a\left(p - j, q + \frac{v}{2}\right) b\left(p + j', q + \frac{v'}{2}\right) \qquad \text{(A8)} \end{aligned}$$

We combine Eqs. (A7) and (A8) and make the following further change of variables,

$$\begin{aligned} p + j' &= p' \\ q + \frac{v'}{2} &= q' \end{aligned} \qquad \text{(A9)}$$

to bring the results into an integral operator form. Noting that the sum and difference of $a(p + j, q - v/2)$ and $a(p - j, q + v/2)$ is "even" and "odd," respectively, in the variables $j$ and $v$, we may therefore now write

$$\sin(\hat{\Lambda})\, a(p, q)\, b(p, q)$$

$$= \frac{1}{(h^4)^2} \int dq'\, dp' \left\{ \int dv\, dj \left[ a\left(p + j, q - \frac{v}{2}\right) \right.\right.$$

$$\left. - a\left(p - j, q + \frac{v}{2}\right) \right] \sin\left[\frac{2j}{\hbar} \cdot (q' - q)\right]$$

$$\left. \times i \sin\left(\frac{p' - p}{\hbar} \cdot v\right) \right\} b(p', q') \tag{A10}$$

$$\cos(\hat{\Lambda})\, a(p, q)\, b(p, q)$$

$$= \frac{1}{(h^4)^2} \int dq'\, dp' \left\{ \int dv\, dj \left[ a\left(p + j, q - \frac{v}{2}\right) + a\left(p - j, q + \frac{v}{2}\right) \right] \right.$$

$$\left. \times \cos\left[\frac{2j \cdot (q' - q)}{\hbar}\right] \cos\left(\frac{p' - p}{\hbar} \cdot v\right) \right\} b(p', q') \tag{A11}$$

We have chosen to write the kernels of the integral operator in Eqs. (A10) and (A11) in the form given by Eqs. (63) and (64) in the text, since in the absence of scattering and collision the integral over $j$ can often be carried out when written in the form given in the text.

## APPENDIX B. THE KADANOFF–BAYM *ANSATZ*

Recently Lipavský *et al.* (LSV)$^{(28)}$ proposed a generalized Kadanoff–Baym (KB) *Ansatz* by writing $G^{\gtrless}$ as a product of two operators, one being the density matrix operator for electrons or holes. The idea is to separate the operator whose Weyl transform gives the Wigner distribution function for electrons or holes. However, we see in Appendix A that in general, granted that the separation can be done, the resulting Weyl transform of $G^{\gtrless}$ will not be a simple product of the Weyl transform of the particle density-matrix operator and that of the Weyl transform of the other operator (obtained by some *ad hoc* choice by LSV). The question then becomes, what is a more accurate way of achieving the separation, so that the Weyl transform is approximated by a simple product of Weyl transforms?

As originally proposed by LSV, the generalized KB *Ansatz* is written, in our notation, as

$$-iG^{\gtrless} = i(G^r p^{\gtrless} - p^{\gtrless} G^a) \tag{B1}$$

where the Weyl transform$^{(17)}$ of $p^{<}$ (electron density-matrix operator) is the Wigner distribution function. We can immediately see that the Weyl transform of $-iG^{<}$ is equal to $A(p, q)\, f_w(p, q)$ plus first-order and higher-order gradient corrections.

A more accurate *Ansatz* can easily be obtained by writing Eq. (B1) as

$$-iG^{\gtrless} = \frac{i}{2}\{G^r, p^{\gtrless}\} - \frac{i}{2}\{p^{\gtrless}, G^a\} \tag{B2}$$

which is clearly equal to $A(p, q)\, p^{\gtrless}(p, q)$ plus second-order and higher-order gradient corrections. Equation (B2) is the generalized KB *Ansatz* referred to in the text; it is more accurate and retains the full symmetry between electrons and holes.

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