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Quantum kinetic equation for the Wigner function and reduction to the Boltzmann transport equation under discrete impurities

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We derive a quantum kinetic equation under discrete impurities for the Wigner function from the quantum Liouville equation. To attain this goal, the electrostatic Coulomb potential is separated into the long- and short-range parts, and the self-consistent coupling with Poisson's equation is explicitly taken into account within the analytical framework. It is shown that the collision integral associated with impurity scattering as well as the usual drift term is derived on an equal footing. As a result, we find that the conventional treatment of impurity scattering under the Wigner function scheme is inconsistent in the sense that the collision integral is introduced in an *ad hoc* way and, thus, the short-range part of the impurity potential is double-counted. The Boltzmann transport equation (BTE) is then derived *without imposing the assumption of random impurity configurations* over the substrate. The derived BTE would be applicable to describe the discrete nature of impurities such as potential fluctuations.

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I. INTRODUCTION

Electron transport properties associated with impurity scattering under inhomogeneous structures such as semiconductor devices have been traditionally studied with the semiclassical Boltzmann transport equation (BTE) coupled self-consistently to Poisson's equation [1,2]. The self-consistent coupling with Poisson's equation is necessary as far as the structure is bounded and inhomogeneous because the carrier density is inherently nonuniform. However, such theoretical approaches based on the BTE are incomplete in some respects, namely, when taking into account the discrete nature of impurities. For instance, the electrostatic Hartree potential determined by Poisson's equation represents the potential under the long-wavelength limit [3], and impurity scattering in the collision integral is evaluated under the implicit assumption of self-averaging over all possible impurity configurations [4–8]. As a result, the traditional framework based on the BTE coupled with Poisson's equation completely ignores the discreteness of impurities and cannot describe the phenomena such as potential fluctuations or, equivalently, multi-ion screening effects [9].

A quantum mechanical approach based on the Wigner function does not resolve the problem described above; the classical electron distribution function is replaced by the Wigner function, and the Hartree potential is replaced by the quantum potential derived from the quantum Liouville equation under the long-wavelength limit [4,10]. The scattering processes are introduced through the collision integral with the same reasoning as that in the BTE [11–14]. Namely, the rate of change of the electron distribution function must be balanced between drift and scattering processes [15–17]. We should also mention that the conventional framework of the Wigner function is inconsistent from both mathematical and physical perspectives: The Wigner function cannot be interpreted as a probability density because it is not positive semidefinite, and the scattering potential of impurities is double-counted in both the drift term through the Hartree potential and the collision integral, as we shall explore in the present paper.

After all, under the traditional framework based on the BTE and the Wigner function schemes, impurity scattering is treated independently from the transport equation because the transition probability due to impurity scattering is evaluated by Fermi's golden rule with the *a priori* screened Coulomb potential. This implicitly implies that impurities are always fully screened by carriers no matter whether the system is in equilibrium or nonequilibrium. In other words, as far as impurity scattering is concerned, the "self-consistent coupling" between the transport equation and Poisson's equation is not actually consistently coupled within the framework.

Of course, the problems associated with the discrete nature of impurities and charged particles have been numerically tackled over the past half century. Under the homogeneous case where Poisson's equation *under the long-wavelength limit* is not required, the direct incorporation of the Coulomb interaction among charged particles in high-temperature plasmas has been made by molecular dynamics (MD). Later, the coupling of MD with the Monte Carlo (MC) method was introduced for semiconductors [18–20]. This approach has been further extended to take into account the exchange interaction among electrons [21] and also applied to the electron-impurity systems [22]. The coupled MC-MD method is indeed able to take into account the potential fluctuations associated with the discreteness of charged particles and impurities. Yet, unfortunately, it is applicable only to homogeneous structures. To apply the MC-MD approach to inhomogeneous structures, which are characteristic of semiconductor devices, the

Coulomb potential has been explicitly separated into the long- and short-range parts so that only the short-range part of the potential is introduced via the MD method, whereas the long-range part is taken into account by the mesh field from Poisson's equation [23].

In reality, the discrete nature of impurities is now playing a crucial role in the state-of-the-art technology associated with electron devices: Because of drastic miniaturization of device size, electron transport is now quasiballistic [24–27], and the discrete nature of doped impurities is manifested in various transport characteristics [28]. In particular, discrete impurities induce local potential fluctuations around impurities. Such potential fluctuations are usually masked by screening carriers and do not show up explicitly in equilibrium under bulk structures. This is why the long-wavelength limit imposed on the electrostatic potential in Poisson's equation is justified under the traditional framework. However, electron devices operate under nonequilibrium conditions, and the semiconductor substrate is strongly inhomogeneous. As a result, screening by free carriers is in most cases incomplete, and potential fluctuations always show up during device operation. This leads to threshold voltage variabilities (called random dopant fluctuations, RDFs for short), which cannot be artificially controlled due to the random nature of impurity configurations [29,30]. Such variabilities in device characteristics are considered to be a dominant factor preventing further miniaturization of the leading-edge electron devices. Many numerical studies on the issues of RDF have been conducted under the fluid approximation, the Drift-Diffusion (DD) scheme, because of computational burden [31–35]. We should mention, however, that a rigorous physical justification based on the transport theory of incorporating the discrete nature of impurities into the DD scheme is still missing. This study also makes a step toward such a goal.

In the present paper, we discuss the quantum and semiclassical transport equations with impurity scattering from two different perspectives: One is about the inconsistency between the kinetic equation for the Wigner function and Poisson's equation that exists in double-counting the impurity scattering potential. The other is about the implementation of the discrete nature of impurities into the BTE framework. These issues may seem to be uncorrelated, but actually, they are intimately linked. The relationship between the self-consistent Hartree potential in the drift term and the scattering potential in the collision integral becomes clearer only if the discrete nature of impurities is explicitly introduced into the kinetic equation. To achieve this goal, we separate the long- and short-range parts of the impurity potential in both the quantum kinetic equation for the Wigner function and Poisson's equation, and, thus, the self-consistent coupling between the two equations is explicitly taken into account within the analytical framework. As a matter of fact, the idea of separating the long- and short-range parts of the Coulomb potential has been used in many areas in physics such as plasma simulations [36] and the density functional theory [37]. The above-mentioned MC-MD scheme applicable to inhomogeneous structures is also based on a similar idea [23,38]. Here we follow the conventional approach; the short-range part of the potential is treated as scattering, and the long-range part is taken into account through Poisson's equation. We show by analytical means that the collision integral and the self-consistent Hartree potential can be naturally *derived* in the quantum kinetic equation on an equal footing. Then the semiclassical BTE is reduced from the quantum kinetic equation *without relying on self-averaging of random impurity configurations*, which is a key ingredient to derive the BTE for impurity scattering under the long-wavelength limit [15,16,39,40]. We would like to stress that the BTE for impurity scattering has been indeed derived before from the Wigner equation of motion *yet under the homogeneous cases* so that the assumption of random impurity configurations was crucial in its derivation [41,42].

The present paper is organized as follows. In Sec. II the Wigner function is defined and explicit separation of impurity potential into the long- and short-range parts is introduced in the theoretical framework. In Sec. III, the quantum kinetic equation for the Wigner function is derived and the physical interpretations of the Hartree potential and scattering potential are presented. In Sec. IV, the coarse-grained Wigner function is introduced to derive the quantum kinetic equation in a closed form. In Sec. V, the BTE applicable to the cases under discrete impurities is derived. Finally, some conclusions are drawn in Sec. VI.

II. WIGNER FUNCTION AND IMPURITY POTENTIAL

The Wigner function is defined by the Wyle transform of the density operator [41,42] and expressed by

$$f(\mathbf{p},\mathbf{R},t)=\int\frac{d^3r}{(2\pi)^3}e^{-i\mathbf{p}\cdot\mathbf{r}}\left\langle\mathbf{R}+\frac{\mathbf{r}}{2}\middle|\hat{\rho}(t)\middle|\mathbf{R}-\frac{\mathbf{r}}{2}\right\rangle, \tag{1}$$

where $\hat{\rho}(t)$ is the density operator of electrons in a semiconductor substrate. In the present study, we assume that electrons are so dilute that these electrons are treated as completely independent of the others and the system is dealt with as a single-electron problem. Hence, the electron density operator is represented by a mixed state such that

$$\hat{\rho}(t)=\frac{1}{\nu}\sum_{\alpha}|\psi_{\alpha}(t)\rangle\langle\psi_{\alpha}(t)|, \tag{2}$$

where ν is the number of electrons, $|\psi_{\alpha}(t)\rangle$ is the single-electron state vector, and the sum is taken over all electrons [43]. $\hat{\rho}(t)$ satisfies the quantum Liouville equation

$$i\frac{\partial\hat{\rho}(t)}{\partial t}=[\hat{H},\hat{\rho}(t)], \tag{3}$$

where $\hat{H}$ is the single-electron Hamiltonian and given by $\hat{H}=\hat{p}^2/(2m)-e\hat{V}$, where $\hat{V}$ is the external potential (operator) including the impurity potential, which is self-consistently coupled with the Poisson equation. In the present paper, units are chosen such that $\hbar\equiv 1$. The quantum kinetic equation for the Wigner function is then derived as

$$\begin{aligned}\left[\frac{\partial}{\partial t}+\frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{R}}\right]f(\mathbf{p},\mathbf{R},t)&=-\frac{e}{i}\int\frac{d^3r\,d^3p'}{(2\pi)^3}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{r}}\\&\quad\times\left[V\left(\mathbf{R}+\frac{\mathbf{r}}{2},t\right)-V\left(\mathbf{R}-\frac{\mathbf{r}}{2},t\right)\right]f(\mathbf{p}',\mathbf{R},t).\end{aligned} \tag{4}$$

The discrete impurity density is approximated by a set of δ functions and expressed by

$$N_d^+(\mathbf{R}) = \sum_{i=1}^{N_I} \delta(\mathbf{R}-\mathbf{R}_i), \tag{5}$$

where $\mathbf{R}_i$ is the position of the ith impurity and N_I is the total number of impurities in the substrate. The external potential $V(\mathbf{R},t)$ in Eq. (4) satisfies Poisson's equation, which is, for later discussion, written by

$$\nabla^2 V = -\frac{e}{\varepsilon_s}\{[N_d^+(\mathbf{R}) - N_{d,\text{long}}^+(\mathbf{R})] + [N_{d,\text{long}}^+(\mathbf{R}) - n(\mathbf{R},t)]\}, \tag{6}$$

where $N_{d,\text{long}}^+(\mathbf{R})$ inserted intentionally on the right-hand side represents the impurity density associated with the long-range part of the impurity Coulomb potential (determined below). $n(\mathbf{R},t)$ is the electron density calculated from the Wigner function by

$$n(\mathbf{R},t) = \int d^3\mathbf{p}\, f(\mathbf{p},\mathbf{R},t). \tag{7}$$

By a proper choice of $N_{d,\text{long}}^+(\mathbf{R})$, Eq. (6) can be split into the following two equations:

$$\nabla^2 V_{\text{long}} = -\frac{e}{\varepsilon_s}[N_{d,\text{long}}^+(\mathbf{R}) - n(\mathbf{R},t)] \tag{8}$$

and

$$\nabla^2 V_{\text{short}} = -\frac{e}{\varepsilon_s}[N_d^+(\mathbf{R}) - N_{d,\text{long}}^+(\mathbf{R})], \tag{9}$$

where V_{long} and V_{short} are the long- and short-range parts of the external potential, respectively, and fulfill the relation $V = V_{\text{long}} + V_{\text{short}}$. We would like to point out that $n(\mathbf{R},t)$ calculated from Eq. (7) is regarded as a long-range quantity since $f(\mathbf{p},\mathbf{R},t)$ is a continuous and smooth function of both $\mathbf{p}$ and $\mathbf{R}$.

The separation of impurity potential into the long- and short-range parts becomes unique when one considers the system in equilibrium under bulk structures where the charge neutrality condition also holds [3,44]. Then V_{long} reduces to a flat potential because the long-range part of the impurity potential is completely screened by free electrons and an unscreened part of the potential is excluded from V_{long}, owing to the explicit separation of the potential. Hence, the right-hand side of Eq. (8) must vanish in equilibrium, and we obtain

$$N_{d,\text{long}}^+(\mathbf{R}) \approx \sum_{i=1}^{N_I} n_i^{eq}(\mathbf{R}-\mathbf{R}_i). \tag{10}$$

Notice that Eq. (9) is now decoupled from the quantum kinetic equation (4) and closed by itself. This implies that potential modulations induced by screening are self-consistently taken into account by Eqs. (4) and (8). In other words, static screening and dynamical screening are separated under the present framework, and the latter is treated as collective motion through the quantum kinetic equation, Eq. (4). Assuming that the average impurity density is not extremely large, $N_{d,\text{long}}^+$ is given by a sum of the electron density $n_i^{eq}(\mathbf{R}-\mathbf{R}_i)$ modulated around each impurity. Then we may write $V_{\text{short}}(\mathbf{R}) = \sum_{i=1}^{N_I} v_s(\mathbf{R}-\mathbf{R}_i)$ and Eq. (9) reduces to Poisson's equation for a *single* impurity potential v_s,

$$\nabla^2 v_s = -\frac{e}{\varepsilon_s}\big[\delta(\mathbf{R}-\mathbf{R}_i) - n_i^{eq}(\mathbf{R}-\mathbf{R}_i)\big]. \tag{11}$$

Clearly, this equation along with appropriate boundary conditions leads to the (static) screened Coulomb potential due to a single impurity at position $\mathbf{R}_i$. When we solve Eq. (11) under the linear approximation for unbounded bulk structure, the usual Yukawa potential is derived [45].

III. QUANTUM KINETIC EQUATION FOR THE WIGNER FUNCTION

We now derive the quantum kinetic equation for the Wigner function *under discrete impurities*. The source term, given by the right-hand side of Eq. (4), could be split into two terms in accordance with the long- and short-range parts of the potential, and we may rewrite Eq. (4) as

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{R}}\right) f(\mathbf{p},\mathbf{R},t) = S_{\text{long}}(\mathbf{p},\mathbf{R},t) + S_{\text{short}}(\mathbf{p},\mathbf{R},t), \tag{12}$$

where S_{long} and S_{short} represent the source terms associated with V_{long} and V_{short}, respectively.

A. Long-range part of the source term

The long-range part of the source term is treated in the usual manner [46]. Expanding V_{long} in $S_{\text{long}}(\mathbf{p},\mathbf{R},t)$ around $\mathbf{R}$ by the Taylor series, we find

$$S_{\text{long}}(\mathbf{p},\mathbf{R},t) = -2e\sin\left[\frac{1}{2}\left(\frac{\partial^{(V)}}{\partial \mathbf{R}}\cdot\frac{\partial^{(f)}}{\partial \mathbf{p}} - \frac{\partial^{(V)}}{\partial \mathbf{p}}\cdot\frac{\partial^{(f)}}{\partial \mathbf{R}}\right)\right] \times V_{\text{long}}(\mathbf{R}) f(\mathbf{p},\mathbf{R},t), \tag{13}$$

where $\sin(\cdot)$ is a short-hand notation of its infinite series, and the first and second derivatives inside the argument act on V_{long} and f, respectively.

Notice that this result is exact and no approximation has been made. In the present paper, impurity scattering is our main concern so that V_{long} is independent of the electron's momentum. Therefore, the second term inside the argument of the sin function has essentially no effect. However, it is critical to keep this term in Eq. (13) for being equivalent to the Poisson bracket of Eq. (3), namely,

$$S_{\text{long}}(\mathbf{p},\mathbf{R},t) = \int \frac{d^3r}{(2\pi)^3} e^{-i\mathbf{p}\cdot\mathbf{r}} \left\langle \mathbf{R}+\frac{\mathbf{r}}{2}\right| i[e\hat{V}_{\text{long}},\hat{\rho}(t)] \left|\mathbf{R}-\frac{\mathbf{r}}{2}\right\rangle. \tag{14}$$

Of course, it plays a key role when the Lorentz force associated with magnetic field is involved. Also, we should mention that the higher-order terms above the lowest-order in Eq. (13) lead to the renormalization effects of the electronic states in a similar manner to those found in the Kadanoff-Baym equation [47,48].

B. Short-range part of the source term

Since the length-scale dominant in $S_{\text{short}}(\mathbf{p},\mathbf{R},t)$ is in the opposite limit of $S_{\text{long}}(\mathbf{p},\mathbf{R},t)$, it is more convenient to work in the Fourier-Laplace space, rather than in the real space. The Fourier-Laplace-transform of S_{short} is expressed by

$$\begin{aligned}\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega) &= -\frac{e}{i}\int \frac{d^3q}{(2\pi)^3}\tilde{V}_{\text{short}}(\mathbf{q})\bigg[\tilde{f}\Big(\mathbf{p}-\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\\ &\quad -\tilde{f}\Big(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\bigg], \qquad (15)\end{aligned}$$

where $\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega)$ and $\tilde{V}_{\text{short}}(\mathbf{q})$ are, respectively, defined by

$$\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega) = \int_0^\infty dt \int d^3R e^{-i\mathbf{k}\cdot\mathbf{R}+i\omega t} S_{\text{short}}(\mathbf{p},\mathbf{R},t) \qquad (16)$$

and

$$\tilde{V}_{\text{short}}(\mathbf{q}) = \int d^3R e^{-i\mathbf{q}\cdot\mathbf{R}} V_{\text{short}}(\mathbf{R}). \qquad (17)$$

Equation (12) is formally solved in the Fourier-Laplace space using the Green function. The Wigner function is then given by

$$\begin{aligned}\tilde{f}(\mathbf{p},\mathbf{k},\omega) &= if(\mathbf{p},\mathbf{k},t=0) + G^+(\mathbf{p},\mathbf{k},\omega)\\ &\quad \times i[\tilde{S}_{\text{long}}(\mathbf{p},\mathbf{k},\omega)+\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega)], \qquad (18)\end{aligned}$$

where $G^+(\mathbf{p},\mathbf{k},\omega)$ is the retarded Green function and defined by

$$G^+(\mathbf{p},\mathbf{k},\omega) = \frac{1}{\omega + i\varepsilon - \mathbf{p}\cdot\mathbf{k}/m}. \qquad (19)$$

Here ε is a positive infinitesimal. Although Eq. (18) is an exact solution, we need to make an approximation to evaluate $\tilde{S}_{\text{short}}$ given by Eq. (15). First, we ignore the effects induced by V_{long} during the transition due to impurity scattering, namely, the intracollisional field effect (ICFE) [49–52]. Hence, the Wigner function in Eq. (15) is approximated by

$$\tilde{f}(\mathbf{p},\mathbf{k},\omega) \approx G^+(\mathbf{p},\mathbf{k},\omega)i\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega). \qquad (20)$$

This approximation may be justified because the collision duration is expected to be short, due to the short-range nature of V_{short}, so that the retardation effect during scattering should be insignificant unless an electric field is extremely large. However, as the impurity density increases, the magnitude of the potential fluctuations associated with the long-range part of impurity potential gets larger. In the depletion regions where no carriers for screening exist, the magnitude of an induced electric field exceeds 1 MV/cm when the average impurity density is 10^{20} cm^{-3} [44]. Therefore, the ICFE could be significant at such high impurity densities. However, a large portion of potential fluctuations is usually masked by carrier screening, and, thus, the ICFE would actually become important only in very limited cases such as under the depletion condition. In addition, we ignore a transient correlation resulting from the initial condition of the Wigner function $f(\mathbf{p},\mathbf{k},t=0)$, because the transport properties driven by the source term of Eq. (12) are our main concerns.

Substitution of Eq. (20) into Eq. (15) leads to the following expression for $\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega)$:

$$\begin{aligned}\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega) &= -e\int\frac{d^3q}{(2\pi)^3}\tilde{V}_{\text{short}}(\mathbf{q})\bigg[G^+\Big(\mathbf{p}-\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\tilde{S}_{\text{short}}\Big(\mathbf{p}-\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\\ &\quad - G^+\Big(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\tilde{S}_{\text{short}}\Big(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{k}-\mathbf{q},\omega\Big)\bigg]. \qquad (21)\end{aligned}$$

This formula plays a similar role to the Lippmann-Schwinger equation in the scattering theory [41,53,54]. Hence, all higher-order effects associated with short-range interaction between electrons and impurities such as multiple scattering are included. Keeping only the second order in $\tilde{V}_{\text{short}}$, which is equivalent to the Born approximation, $\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega)$ is approximated by

$$\begin{aligned}\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega) &\approx \frac{e^2}{i}\int\frac{d^3q d^3q'}{(2\pi)^6}\tilde{V}_{\text{short}}(-\mathbf{q})\tilde{V}_{\text{short}}(\mathbf{q}')\\ &\quad\times\bigg\{G^+\Big(\mathbf{p}+\frac{\mathbf{q}}{2},\mathbf{k}+\mathbf{q},\omega\Big)\bigg[\tilde{f}\Big(\mathbf{p}+\frac{\mathbf{q}-\mathbf{q}'}{2},\mathbf{k}+\mathbf{q}-\mathbf{q}',\omega\Big)-\tilde{f}\Big(\mathbf{p}+\frac{\mathbf{q}+\mathbf{q}'}{2},\mathbf{k}+\mathbf{q}-\mathbf{q}',\omega\Big)\bigg]\\ &\quad - G^+\Big(\mathbf{p}-\frac{\mathbf{q}}{2},\mathbf{k}+\mathbf{q},\omega\Big)\bigg[\tilde{f}\Big(\mathbf{p}-\frac{\mathbf{q}+\mathbf{q}'}{2},\mathbf{k}+\mathbf{q}-\mathbf{q}',\omega\Big)-\tilde{f}\Big(\mathbf{p}-\frac{\mathbf{q}-\mathbf{q}'}{2},\mathbf{k}+\mathbf{q}-\mathbf{q}',\omega\Big)\bigg]\bigg\}. \qquad (22)\end{aligned}$$

C. Quantum kinetic equation

The quantum kinetic equation for the Wigner function is now given by

$$\bigg\{-i\omega+\frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{R}}+2e\sin\bigg[\frac{1}{2}\Big(\frac{\partial^{(V)}}{\partial\mathbf{R}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{p}}-\frac{\partial^{(V)}}{\partial\mathbf{p}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{R}}\Big)\bigg]V_{\text{long}}(\mathbf{R})\bigg\}f(\mathbf{p},\mathbf{R},\omega) = S_{\text{short}}(\mathbf{p},\mathbf{R},\omega), \qquad (23)$$

where $S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)$ is the inverse-Fourier transform of $\tilde{S}_{\text{short}}(\mathbf{p},\mathbf{k},\omega)$ expressed by Eq. (22).

We would like to stress, however, that Eq. (23) is incomplete in the respect that the Fourier transform of $f(\mathbf{p},\mathbf{R},\omega)$ on the left-hand side of Eq. (23) is not consistent with $\tilde{f}(\mathbf{p},\mathbf{k},\omega)$ in $S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)$: The ICFE associated with the (long-range) spatial variation of $V_{\text{long}}(\mathbf{R})$ is ignored in $\tilde{f}(\mathbf{p},\mathbf{k},\omega)$ of $S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)$ because of the approximation employed by Eq. (20). Therefore, the following two important facts must be considered. First, $\tilde{f}(\mathbf{p},\mathbf{k},\omega)$ in Eq. (22) is regarded as the Fourier-Laplace transform of $f(\mathbf{p}, \mathbf{R}, t)$ as if the electrostatic potential were fixed with the "local" value $V_{\text{long}}(\mathbf{R})$ during collision duration. Second, the Markov approximation is inevitable at this stage because $\tilde{f}(\mathbf{p}, \mathbf{k}, \omega)$ of $S_{\text{short}}(\mathbf{p}, \mathbf{R}, \omega)$ is not updated during collision duration consistently with $V_{\text{long}}(\mathbf{R})$. As a result, ω-dependence in the retarded Green function $G^{+}(\mathbf{p}, \mathbf{k}, \omega)$ is decoupled from that of $\tilde{f}(\mathbf{p}, \mathbf{k}, \omega)$ in Eq. (22). In other words, the quantum kinetic equation (23) is not actually closed for the Wigner function, and we need to complement another relation between $f(\mathbf{p}, \mathbf{R}, \omega)$ of the left-hand side of Eq. (23) and $\tilde{f}(\mathbf{p}, \mathbf{k}, \omega)$ in $S_{\text{short}}(\mathbf{p}, \mathbf{R}, \omega)$ of the right-hand side.

IV. KINETIC EQUATION FOR THE COARSE-GRAINED WIGNER FUNCTION

A. Coarse-grained Wigner function

To close the quantum kinetic equation (23) for the Wigner function, we introduce the spatial average (coarse graining) of the Wigner function with respect to the weight function $g(\mathbf{R})$, which is normalized to unity over the space. In fact, coarse graining often has been introduced in past studies to explain the appearance of irreversibility in the transport equations, although in most cases it has been applied to the time or energy domain [39,40]. In the present study, however, we define the coarse-grained Wigner function in space by

$$\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle = \int d^3R' g(\mathbf{R}') f(\mathbf{p}, \mathbf{R} - \mathbf{R}', \omega), \tag{24}$$

and $g(\mathbf{R})$ is assumed to have the following expression:

$$g(\mathbf{R}) = \frac{{q_c}^3}{(2\pi)^{3/2}} e^{-\frac{{q_c}^2\mathbf{R}^2}{2}}. \tag{25}$$

Here q_c is the inverse of the screening length determined by Poisson's equation for the short-range part of the potential, as given by Eq. (11). Since q_c is dependent on the modulated electron density $n_i^{eq}(\mathbf{R} - \mathbf{R}_i)$ around the impurity at $\mathbf{R}_i$, it is also dependent on $\mathbf{R}$ through $V_{\text{long}}(\mathbf{R})$. Notice that Eq. (24) is also expressed by

$$\begin{aligned}\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{R}} \tilde{g}(\mathbf{k}) \tilde{f}(\mathbf{p}, \mathbf{k}, \omega) \\ &\approx \frac{1}{\Delta\Omega_{\mathbf{R}}} \tilde{f}(\mathbf{p}, \mathbf{k} = 0, \omega),\end{aligned} \tag{26}$$

where in the last line we used the fact that $\tilde{g}(\mathbf{k})$ is given by $\tilde{g}(\mathbf{k}) = \exp(-\mathbf{k}^2/2{q_c}^2)$ and sharply peaked at $\mathbf{k} = 0$. $\Delta\Omega_{\mathbf{R}}$ is the volume with the screening length q_c^{-1} and given by $\Delta\Omega_{\mathbf{R}} = (2\pi)^{3/2}/{q_c}^3$ and, thus, $\Delta\Omega_{\mathbf{R}}$ also becomes dependent on position $\mathbf{R}$ through q_c^{-1}. It is clear from Eq. (26) that $\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle$ is indeed the Wigner function averaged over the (macroscopically small) volume at $\mathbf{R}$. As a result, $\tilde{f}(\mathbf{p}, \mathbf{k} = 0, \omega)$ is diagonal in momentum space and $\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle$ becomes positive semidefinite. Furthermore, as seen from Eq. (24), $\tilde{f}(\mathbf{p}, \mathbf{k} = 0, \omega)$ is the Fourier transform of the Wigner function centered at the position $\mathbf{R}$. Hence, $\tilde{f}(\mathbf{p}, \mathbf{k} = 0, \omega)$ may be regarded as the Fourier-transformed Wigner function that is obtained under the assumption as if the electrostatic potential were fixed with the value of $V_{\text{long}}(\mathbf{R})$ over the volume Ω. This is exactly the same interpretation employed for the Fourier-transformed Wigner function in $S_{\text{short}}(\mathbf{p}, \mathbf{R}, \omega)$ of Eq. (23). Therefore, Eq. (26) plays a complementary relation to close Eq. (23).

B. Quantum kinetic equation in a closed form

We now impose the spatial average on both sides of Eq. (23). Noting that the operation of space differentiation commutes with the averaging operation, we immediately obtain

$$\left(-i\omega + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{R}}\right)\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle + 2e \sin\left[\frac{1}{2}\left(\frac{\partial^{(V)}}{\partial \mathbf{R}} \cdot \frac{\partial^{(f)}}{\partial \mathbf{p}} - \frac{\partial^{(V)}}{\partial \mathbf{p}} \cdot \frac{\partial^{(f)}}{\partial \mathbf{R}}\right)\right]\langle V_{\text{long}}(\mathbf{R}) f(\mathbf{p}, \mathbf{R}, \omega)\rangle = \langle S_{\text{short}}(\mathbf{p}, \mathbf{R}, \omega)\rangle. \tag{27}$$

Notice that $V_{\text{long}}(\mathbf{R})$ varies in space with the length scale greater than q_c^{-1}, whereas the space average is taken over the region smaller than q_c^{-1}. Hence, the space averaging of $V_{\text{long}}(\mathbf{R})$ has little effect, and we can approximate

$$\langle V_{\text{long}}(\mathbf{R}) f(\mathbf{p}, \mathbf{R}, \omega)\rangle \approx V_{\text{long}}(\mathbf{R})\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle. \tag{28}$$

On the other hand, the right-hand side of Eq. (27) becomes

$$\begin{aligned}\langle S_{\text{short}}(\mathbf{p}, \mathbf{R}, \omega)\rangle = \frac{e^2}{i} \frac{1}{\Omega^2} \sum_{\mathbf{q},\mathbf{q}'} \tilde{V}_{\text{short}}(-\mathbf{q}) \tilde{V}_{\text{short}}(\mathbf{q}') \frac{1}{\Delta\Omega_{\mathbf{R}}} \bigg\{ G^{+}\left(\mathbf{p} + \frac{\mathbf{q}}{2}, \mathbf{q}, \omega\right)\left[\tilde{f}\left(\mathbf{p} + \frac{\mathbf{q} - \mathbf{q}'}{2}, \mathbf{q} - \mathbf{q}', \omega\right)\right. \\ \left. - \tilde{f}\left(\mathbf{p} + \frac{\mathbf{q} + \mathbf{q}'}{2}, \mathbf{q} - \mathbf{q}', \omega\right)\right] - G^{+}\left(\mathbf{p} - \frac{\mathbf{q}}{2}, \mathbf{q}, \omega\right)\left[\tilde{f}\left(\mathbf{p} - \frac{\mathbf{q} + \mathbf{q}'}{2}, \mathbf{q} - \mathbf{q}', \omega\right) - \tilde{f}\left(\mathbf{p} - \frac{\mathbf{q} - \mathbf{q}'}{2}, \mathbf{q} - \mathbf{q}', \omega\right)\right]\bigg\},\end{aligned} \tag{29}$$

where Ω is the volume of the substrate and integral over the momentum is now replaced by the sum by following the box normalization rule. Also, the following relationship is used;

$$\langle e^{i\mathbf{k}\cdot\mathbf{R}}\rangle = e^{i\mathbf{k}\cdot\mathbf{R}} \tilde{g}(\mathbf{k}). \tag{30}$$

Because of Eq. (26), $\langle f(\mathbf{p}, \mathbf{R}, \omega)\rangle$ on the left-hand side of Eq. (27) is diagonal in momentum space and, thus, Eq. (29) is singular with respect to the diagonal components of $\tilde{f}(\mathbf{p}, \mathbf{k}, \omega)$ [55]. Hence, we may write

$$\tilde{f}\left(\mathbf{p} \pm \frac{\mathbf{q} \pm \mathbf{q}'}{2}, \mathbf{q} - \mathbf{q}', \omega\right) \approx \delta_{\mathbf{q},\, \mathbf{q}'} \tilde{f}\left(\mathbf{p} \pm \frac{\mathbf{q} \pm \mathbf{q}}{2}, 0, \omega\right). \tag{31}$$

Notice that ω-dependence of $G^{+}(\mathbf{p},\mathbf{q},\omega)$ represents the energy change during collision duration due to impurity scattering, whereas that of $\tilde{f}(\mathbf{p},\mathbf{k},\omega)$ represents the energy change during an electron's drift motion induced by the left-hand side of Eq. (27). Therefore, ω-dependences of $G^{+}(\mathbf{p},\mathbf{q},\omega)$ and $\tilde{f}(\mathbf{p},\mathbf{k},\omega)$ are not correlated with each other, as discussed in Sec. III C. Hence, we may set $\omega = 0$ in $G^{+}(\mathbf{p},\mathbf{q},\omega)$ because impurity scattering is static, and we obtain

$$G^{+}\left(\mathbf{p}\pm\frac{\mathbf{q}}{2},\mathbf{q},\omega=0\right) = \frac{1}{i\varepsilon \mp (E_{\mathbf{p}\pm\mathbf{q}} - E_{\mathbf{p}})} \xrightarrow{\varepsilon\to 0^{+}} \mp P\frac{1}{E_{\mathbf{p}\pm\mathbf{q}} - E_{\mathbf{p}}} - i\pi\delta(E_{\mathbf{p}\pm\mathbf{q}} - E_{\mathbf{p}}), \tag{32}$$

where $E_{\mathbf{p}}$ is an electron's energy with momentum $\mathbf{p}$. Consequently, the coarse-grained source term $\langle S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)\rangle$ is given by

$$\langle S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)\rangle = 2\pi\frac{e^{2}}{\Omega^{2}}\sum_{\mathbf{q}}|\tilde{V}_{\text{short}}(\mathbf{q})|^{2}\delta(E_{\mathbf{p}\pm\mathbf{q}} - E_{\mathbf{p}}) \times \frac{1}{\Delta\Omega_{\mathbf{R}}}[\tilde{f}(\mathbf{p}+\mathbf{q},0,\omega) - \tilde{f}(\mathbf{p},0,\omega)]. \tag{33}$$

Using Eq. (26), the quantum kinetic equation (23) is now closed for the coarse-grained Wigner function $\langle f(\mathbf{p},R,\omega)\rangle$, and we obtain

$$\left\{-i\omega + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{R}} + 2e\sin\left[\frac{1}{2}\left(\frac{\partial^{(V)}}{\partial\mathbf{R}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{p}} - \frac{\partial^{(V)}}{\partial\mathbf{p}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{R}}\right)\right]V_{\text{long}}(\mathbf{R})\right\}\langle f(\mathbf{p},\mathbf{R},\omega)\rangle = \sum_{\mathbf{q}}W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q})[\langle f(\mathbf{p}+\mathbf{q},\mathbf{R},\omega)\rangle - \langle f(\mathbf{p},\mathbf{R},\omega)\rangle], \tag{34}$$

where the transition probability $W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q})$ between an electron's momentum $\mathbf{p}$ and $\mathbf{p}+\mathbf{q}$ via short-range impurity scattering is defined by

$$W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q}) = 2\pi\frac{1}{\Omega^{2}}|e\tilde{V}_{\text{short}}(\mathbf{q})|^{2}\delta(E_{\mathbf{p}+\mathbf{q}} - E_{\mathbf{p}}). \tag{35}$$

The square of the scattering potential is expressed by

$$\frac{1}{\Omega^{2}}|e\tilde{V}_{\text{short}}(\mathbf{q})|^{2} = \frac{1}{\Omega^{2}}|e\tilde{v}_{s}(\mathbf{q})|^{2}\sum_{i=1}^{N_I}\left(1 + \sum_{j\neq i}^{N_I}e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\right) \approx \frac{\bar{n}_{\text{imp}}}{\Omega}|e\tilde{v}_{s}(\mathbf{q})|^{2}, \tag{36}$$

where we used the fact that the zero-Fourier component of $\tilde{v}_{s}(\mathbf{q})$ is already excluded so that the phase interference among multiple impurities represented by the second term inside the bracket of the second line is negligible. $\bar{n}_{\text{imp}}$ is the average impurity density and is defined by $\bar{n}_{\text{imp}} = N_I/\Omega$. Then Eq. (36) exactly coincides with the expression used for impurity scattering under the conventional Wigner function framework.

This expression is, however, inappropriate under discrete impurities. Noting that

$$\frac{1}{\Omega}e\tilde{V}_{\text{short}}(\mathbf{q}) = \frac{1}{\Omega}\int_{\Omega}d^{3}R\,e^{-i\mathbf{q}\cdot\mathbf{R}}eV_{\text{short}}(\mathbf{R}) = \langle\mathbf{p}+\mathbf{q}|e\hat{V}_{\text{short}}|\mathbf{p}\rangle, \tag{37}$$

the transition matrix associated with the short-range impurity potential is evaluated by electron's plane wave $\langle\mathbf{R}|\mathbf{p}\rangle = e^{i\mathbf{R}\cdot\mathbf{p}}/\sqrt{\Omega}$, which spreads over the entire substrate Ω. On the other hand, the transition probability $W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q})$ is derived from $\langle S_{\text{short}}(\mathbf{p},\mathbf{R},\omega)\rangle$ under the assumption that the electrostatic potential is fixed with a "local" value $V_{\text{long}}(\mathbf{R})$ during collision duration. Hence, Eq. (36) should be interpreted only locally in space. Namely, we may regard it as the transition probability obtained for the case as if impurities were distributed over the substrate consistently with the "local" long-range potential $V_{\text{long}}(\mathbf{R})$. As a result, N_I in Eq. (36) is replaced by $N^{+}_{d,\text{long}}(\mathbf{R}) \times \Omega$ and Eq. (35) becomes

$$W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q}) = 2\pi N^{+}_{d,\text{long}}(\mathbf{R})\frac{1}{\Omega}|e\tilde{v}_{s}(\mathbf{q})|^{2}\delta(E_{\mathbf{p}+\mathbf{q}} - E_{\mathbf{p}}). \tag{38}$$

The quantum kinetic equation derived here is nearly identical to the one widely used for quantum transport simulations for semiconductor nanostructures under the Wigner function scheme [10–14]. Yet there are a few critical differences between the present theory and the conventional Wigner function scheme: One is in the drift term of the left-hand side of Eq. (34), in which the whole external potential $V(\mathbf{R})$ in the conventional scheme is now replaced by $V_{\text{long}}(\mathbf{R})$. Hence, as mentioned earlier, the self-consistent Hartree potential is given by $V_{\text{long}}(\mathbf{R})$, rather than $V(\mathbf{R})$. Another point is that the collision integral associated with $V_{\text{short}}(\mathbf{R})$ is naturally *derived* from the quantum Liouville equation in the present theory. Therefore, the double-counting of the short-range scattering potential is eliminated under the present framework. Furthermore, the Wigner function in the conventional scheme is now replaced by the coarse-grained Wigner function. Although the Wigner function can be negative where quantum phase interference is significant, the coarse-grained Wigner function is always positive semidefinite, and, thus, it can be interpreted as a probability density.

V. REDUCTION TO THE BOLTZMANN TRANSPORT EQUATION

The reduction of Eq. (34) to the BTE is straightforward. Since $V_{\text{long}}(\mathbf{R})$ varies gradually in space, the first term of the series on the left-hand side of Eq. (34) is most significant. Keeping only the lowest-order term, we obtain the drift term, which is similar to the expression of the BTE with no magnetic field;

$$2e\sin\left[\frac{1}{2}\left(\frac{\partial^{(V)}}{\partial\mathbf{R}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{p}}-\frac{\partial^{(V)}}{\partial\mathbf{p}}\cdot\frac{\partial^{(f)}}{\partial\mathbf{R}}\right)\right]V_{\text{long}}(\mathbf{R})$$

$$\times\langle f(\mathbf{p},R,\omega)\rangle\approx e\frac{\partial V_{\text{long}}(\mathbf{R})}{\partial\mathbf{R}}\cdot\frac{\partial}{\partial\mathbf{p}}\langle f(\mathbf{p},R,\omega)\rangle. \quad (39)$$

This simply reflects the fact that quantum phase interference between the incident and reflected waves induced by $V_{\text{long}}(\mathbf{R})$ is ignored because of gradual variations of the potential. It should be pointed out, however, that this approximation breaks down if the whole potential $V(\mathbf{R})$, instead of $V_{\text{long}}(\mathbf{R})$, is used as the Hartree potential. Consequently, Eq. (34) reduces to the BTE,

$$\left[-i\omega+\frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{R}}+e\frac{\partial V_{\text{long}}(\mathbf{R})}{\partial\mathbf{R}}\cdot\frac{\partial}{\partial\mathbf{p}}\right]\langle f(\mathbf{p},R,\omega)\rangle$$

$$=\sum_{\mathbf{q}}W_{\text{imp}}(\mathbf{p},\mathbf{p}+\mathbf{q})[\langle f(\mathbf{p}+\mathbf{q},R,\omega)\rangle-\langle f(\mathbf{p},R,\omega)\rangle]. \quad (40)$$

Although the above BTE is almost identical to the conventional BTE with impurity scattering, we should regard it as an extended version of the BTE applicable to discrete impurities. Since $V_{\text{long}}(\mathbf{R})$ is self-consistently coupled with Poisson's equation, the discrete nature of impurities could be represented as potential fluctuations when the screening of impurities by electrons is incomplete. Furthermore, the transition probability due to impurities is evaluated by the *local* impurity density $N^+_{d,\text{long}}(\mathbf{R})$, rather than the average impurity density $\bar{n}_{\text{imp}}(\mathbf{R})$. Therefore, impurity scattering becomes localized around impurities, and the discreteness of impurities is also reflected in the collision integral. Last, yet most importantly, the present derivation has been possible only because we do not rely on self-averaging over the random impurity configurations.

The validity of the derived kinetic equation has been confirmed by applying it to the MC simulations under bulk structures, in which impurities are distributed at random over a Si substrate [56]. We have confirmed that the simulated electron mobility is insensitive to the details of impurity configurations due to self-averaging, although impurity scattering is strongly localized in the present scheme. Furthermore, electron mobilities at various impurity densities coincide very well with the results obtained under the conventional MC simulations with "jellium" impurity in which impurity scattering is delocalized.

Finally, we would also like to mention that a similar treatment can be applied to the long-range part of the Coulomb interaction among electrons. In such cases, the Coulomb interaction induces "dynamical" potential fluctuations, namely, plasma oscillations [57–59], and those collective motions are taken into account through the Poisson equation in a self-consistent manner, rather than the dynamical dielectric function of the scattering potential. This is also consistent with the fact that the plasma oscillation among electrons results from the long-range part of the Coulomb potential $V_{\text{long}}(\mathbf{R})$.

VI. CONCLUSION

We have derived a quantum kinetic equation for the Wigner function under discrete impurities from the quantum Liouville equation in a closed form. This has been achieved by explicitly separating the electrostatic Coulomb potential into the long- and short-range parts and taking into account the self-consistent coupling with Poisson's equation. We have shown that the collision integral associated with impurity scattering as well as the usual drift term is *derived* on an equal footing. Hence, the conventional treatment of impurity scattering under the Wigner function scheme is inconsistent because the collision integral is introduced in an *ad hoc* way and the short-range part of the impurity potential is double-counted. Furthermore, introducing the coarse-grained Wigner function in space, the quantum kinetic equation reduces to a closed form with the coarse-grained Wigner function and becomes consistent with the approximations implicitly imposed on the kinetic equation. Also, the Wigner function becomes positive semidefinite and, thus, can be interpreted as a probability density in the present framework. The BTE has been derived without imposing the long-wavelength limit of the Hartree potential and the self-averaging over random impurity configurations, which have been essential ingredients to *derive* the BTE with impurity scattering under bulk structures. The derived BTE is able to take into account the discrete nature of impurities and applicable to the analysis of electron transport under semiconductor nanostructures.

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