Quantum transport for a Bloch electron quasiparticle in an inhomogeneous electric field scattering from a random distribution of impurities: A Wigner approach

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The quantum transport equation is derived in terms of the Wigner distribution function for a Bloch electron quasiparticle, that is, a Bloch electron in a single band, interacting with a random, inhomogeneous distribution of impurities, and subject to general homogeneous and inhomogeneous electric fields. The time dependent homogeneous electric field is described through the vector potential gauge. The derivation of the transport equation makes use of a unitary transformation of the Liouville equation based on the interaction picture to a form in which the scattering interaction appears quadratically, and utilizes accelerated Bloch states as basis states; the resulting generalized drift and diffusion terms are obtained exactly for an arbitrary band structure. In taking the limit of slowly varying inhomogeneous electric field and slowly varying scatterer density distribution, a quantum generalization of the Boltzmann-like Wigner transport equation is obtained which includes impurity-related intracollisional field effects in the collision term and a drift term comprising the total force due to both the homogeneous and inhomogeneous fields.

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I. INTRODUCTION

In the initial work of Bloch,[1] transport phenomena in solids had been analyzed by employing the Boltzmann transport equation (BTE) in which the electrons were treated as quasiparticles with their energy dispersion relation given by the energy band functions of the unperturbed crystal. A quantum-mechanical derivation of this transport equation had been provided by Kohn and Luttinger[2] (KL) for Bloch electrons interacting with randomly distributed static impurities moving in the presence of a homogeneous electric field in the low field limit; they showed that under these conditions, it followed from the Liouville equation that the diagonal elements of the density matrix, that is, the distribution function in the Bloch representation, satisfied a linearized BTE. The work of KL was later extended by Argyres[3] to include electron-phonon scattering.

The extension of these theories to a derivation of a quantum transport equation (QTE) that is valid for homogeneous fields of arbitrary strength and time dependence has been given by Levinson[4] and Barker[5] who showed, using an effective Hamiltonian which described the electrons in the effective mass approximation, that the scattering term in the QTE included the effect of the field, the so-called intracollisional field effect (ICFE). Calecki and Pottier,[6] using a theorem of Levinson,[4] have shown that these results can be easily extended to Bloch electrons moving in a single band and interacting with phonons by employing an accelerated Bloch state representation (ABR) with basis states that are instantaneous eigenfunctions of the Hamiltonian in which the electric field is described by a vector potential. This representation, which employs Houston-like[7] functions as basis states, has also been used to give a more rigorous analysis of Bloch electron dynamics in the presence of homogeneous electric fields,[8] including tunneling effects, than is possible when the field is described by a scalar potential. Later, using the ABR, Krieger and Iafrate[9] extended the results of Calecki and Pottier to the multiband case for both impurities scattering and phonon scattering; these results include the effects of interband (Zener) tunneling, field-dependent scattering matrix elements, and interband coherent impurity scattering in the QTE in addition to the ICFE.

A second class of problems, in which the quantum-mechanical extension of the BTE has been studied, concerns the interaction of electrons with inhomogeneous fields. In this case, due to the quantum-mechanical nature of the electron, it is not possible to define a function that gives the simultaneous probability density to find an electron at $\boldsymbol{r}$ with momentum $\hbar\boldsymbol{k}$ as is assumed in the classical BTE. However, Wigner[10] has shown that it is possible to define a quantum-mechanical generalization of the classical distribution function such that when integrated over $\boldsymbol{r}$ yields the momentum probability density and when integrated over $\boldsymbol{k}$ yields the probability density in configuration space. Many[11] have stressed the need for a QTE for the Wigner function in order to understand transport in ultrasubmicron devices.

The earliest work in deriving a QTE for electrons moving in a single band and interacting with inhomogeneous fields and elastic scattering has been given by Price[12] who considered an electric field with a single Fourier component in wavelength and frequency. He finds, using an extension of the KL method, that in the large wavelength limit the QTE contains the usual diffusion term found in the BTE, but for electric fields of finite wavelength, quantum correlations appear. Subsequently, Charbonneau *et al.*[13] had provided a derivation of a QTE for the Wigner function by employing many-body linear response theory in a one band model for elastic scattering. As in the work of Price, their analysis is restricted to the low field limit.

In recent years, much progress has been forged in developing the Wigner approach to quantum transport—extensive discussion of dissipative processes and open boundary conditions;[14] first-principle derivations of generalized Wigner function to include electron-phonon interactions;[15,16] the use of advanced numerical schemes and analysis;[17] and a treatment of invariant formulations and gauge equivalence.[18] A recent insightful discourse on the Wigner-Boltzmann transport equation, along with a comprehensive and updated list of references to a wide variety of theoretical and modeling papers, can be found in the work of Nedjalkov *et al.*[19]

In the present work, the QTE is derived for a Bloch electron quasiparticle in a single band interacting with a random, inhomogeneous distribution of impurities, and is subject to general superimposed homogeneous and inhomogeneous fields. The equation for the Wigner distribution function is derived from the Liouville equation; the electrons are described by an effective Hamiltonian interacting with a random, but inhomogeneous distribution of elastic scatterers in the simultaneous presence of an inhomogeneous time-dependent potential and a homogeneous electric field of arbitrary magnitude and time dependence. This particular formulation allows for the analysis of the role of such inhomogenities in disrupting Bloch oscillations from first principles;[20] the inclusion of multiband Zener tunneling in affecting Bloch oscillations can be found elsewhere.[9] More generally, this formulation is applicable to the modeling of an interesting class of high-field transport problems in nanostructures such as modulation-doped semiconductors (e.g., *nipi*'s), inhomogeneously doped heterostructures (HEMTs), and scaled ultrasubmicron complementary metal-oxide semiconductor (CMOS) devices, where inhomogeneities and quantum effects are prevalent. Of course, this approach is not limited to conventional three-dimensional analysis, so it can be readily adapted for emerging low-dimensional applications.

In Sec. II, it is shown that the Liouville equation can be transformed exactly by means of a unitary transformation based on the interaction picture to a form in which the scattering interaction appears quadratically; utilization of this form of the Liouville equation is discussed and is seen to be central in obtaining an approximate closed expression for the diagonal elements of the density matrix without necessarily treating the off-diagonal elements as small due to weak scattering. In Sec. III, the matrix elements of the transformed Liouville equation are evaluated using as basis states the instantaneous eigenstates of the single band effective Hamiltonian which includes the homogeneous electric field through the use of the vector potential gauge. The equation for the Wigner distribution function is derived from the transformed Liouville equation; the generalized drift and diffusion terms are obtained exactly for arbitrary band structure, and the collision integral is obtained to second order in the strength of the scattering potential, the only approximation being the neglect of the inhomogeneous potential in the evaluation of the scattering matrix elements. In Sec. IV, the results are shown to reduce to previously obtained quantum transport equations in the limit in which the inhomogeneous potential is absent and the impurities are homogeneously distributed. Results are also shown to reduce to a quantum generalization of the Boltzmann-like equation in the limit in which the inhomogeneous potential and impurity distribution vary slowly over the de Broglie wavelength; here, the collision term neglects the inhomogeneous field dependence, but includes an impurity related intracollisional field effect and a drift term with the total force comprising the homogeneous and inhomogeneous fields.

II. TRANSFORMATION OF THE LIOUVILLE EQUATION

The Liouville equation for the one electron density matrix operator $\hat{\rho}(t)$ is

$$i\hbar\frac{\partial\hat{\rho}}{\partial t}=[\hat{H}+\hat{H}',\hat{\rho}]. \tag{1}$$

Here the total Hamiltonian for a single electron consists of $\hat{H}(t)$ representing the Hamiltonian for the unperturbed system, such as the effective Hamiltonian for Bloch electron including both the homogeneous and inhomogeneous fields, and the interaction part $\hat{H}'(t)$, in our case, representing an effect of impurities. If, in the spirit of the interaction picture, we subject the Liouville equation in Eq. (1) to a unitary transformation $\hat{U}$ defined by

$$i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t}=\hat{H}(t)\hat{U}(t,t_0), \tag{2}$$

where $\hat{U}(t,t)\equiv\hat{\mathbb{1}}$ for arbitrary t, so that Eq. (2) can also be rewritten in the integral form as

$$\hat{U}(t,t_0)=\hat{\mathbb{1}}-\frac{i}{\hbar}\int_{t_0}^{t}dt'\hat{H}(t')\hat{U}(t',t_0), \tag{3}$$

then, from Eqs. (1) and (2), we see that

$$i\hbar\frac{\partial}{\partial t}(\hat{U}^{+}\hat{\rho}\hat{U})=\hat{U}^{+}[\hat{H}',\hat{\rho}]\hat{U}. \tag{4}$$

It follows, after integrating Eq. (4) over time and using the unitary property $\hat{U}^{+}\hat{U}=\hat{U}\hat{U}^{+}\equiv\hat{\mathbb{1}}$, as well as $\hat{U}(t,t')\hat{U}(t',t_0)=\hat{U}(t,t_0)$, that

$$\hat{\rho}(t)=\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}(t_0,t)-\frac{i}{\hbar}\int_{t_0}^{t}dt'\hat{U}(t,t')\times[\hat{H}'(t'),\hat{\rho}(t')]\hat{U}(t',t). \tag{5}$$

Putting $\hat{\rho}$ of Eq. (5) into the right-hand side of Eq. (1) results in

$$i\hbar\frac{\partial\hat{\rho}}{\partial t}=[\hat{H},\hat{\rho}]+[\hat{H}'(t),\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}(t_0,t)]-\frac{i}{\hbar}\left[\hat{H}'(t),\int_{t_0}^{t}dt'\hat{U}(t,t')[\hat{H}'(t'),\hat{\rho}(t')]\hat{U}(t',t)\right]. \tag{6}$$

Equation (6) is an exact consequence of Eqs. (1) and (2). The prescribed unitary transformation of Eq. (2) has separated the

interaction contribution of the Liouville equation in Eq. (6) into two components; the first component is linear in the interaction term, and is characterized by the time evolution of the initial condition; the second term is quadratic in the interaction term, and contains explicit quantum correlations of $\hat{\rho}$ with $\hat{H}'$, along with temporal memory effects.

No doubt, Eq. (6) appears to be significantly more complicated than Eq. (1) from which it was derived, so its value might be questionable. In order to appreciate the utility of the transformed Liouville equation, we note that if we consider the free electron case, in which there is no inhomogeneous potential, taking the diagonal matrix elements of Eq. (6) with the instantaneous eigenfunctions of $\hat{H}$, assuming that $\hat{\rho}$ is diagonal in this representation at $t=t_0$ before the field is turned on, leads immediately to a QTE in the accelerated Bloch state representation. This follows from the fact that if $\hat{\rho}$ is diagonal at $t=t_0$ in this representation, the diagonal matrix elements of the term in Eq. (6) that involves $\hat{\rho}(t_0)$ are zero. The resulting equation then has the same form as considered by Calecki and Pottier[6] for the case of electron-phonon scattering and can be written in terms of matrix elements of $\hat{H}$ and $\hat{\rho}$ by inserting complete sets of states between products of operators. In the case studied by Calecki and Pottier, the resulting equation is a *closed equation* for the diagonal elements of $\hat{\rho}$ because, for electron-phonon scattering, the $\boldsymbol{k}$ selection rules lead to only diagonal elements of $\hat{\rho}$ in the scattering term. Analogously, in the case of randomly distributed elastic scatterers, taking the ensemble average of the diagonal element of Eq. (6) leads to a closed equation for the diagonal elements of the distribution function which is identical to that previously obtained by Krieger and Iafrate,[9] once we employ the fact that[12]

$$\langle H'_{\boldsymbol{K}\boldsymbol{K}'} H'_{\boldsymbol{K}'\boldsymbol{K}''} \rangle = 0 \quad \text{for } \boldsymbol{K} \neq \boldsymbol{K}''. \tag{7}$$

Similar considerations, assuming a one band model as done by Calecki and Pottier for electron-phonon scattering, also yield the same type of closed equation in the diagonal elements of $\hat{\rho}$ as obtained in Ref. 9 for the case of elastic scatterers randomly distributed on a lattice.

These illustrative examples demonstrate that Eq. (6) is a useful transformation of the Liouville equation and leads directly to a QTE identical to that obtained using the KL method, *without the need* to employ the KL method *of treating the off-diagonal elements of the density matrix as small due to weak scattering*. This is of particular interest when we consider the additional effect of an inhomogeneous potential because a free (or Bloch) electron can have its state changed by interaction with such a potential which can lead to large off-diagonal matrix elements of $\hat{\rho}$ which we would like to treat as exactly as possible. However, the fact that we get the same equation for the distribution function as obtained in Ref. 9, in which the equation for the distribution function was derived in the lowest nonvanishing order in λ, the strength of the electron-scatterer interaction, is at first somewhat surprising. But this comes about because it is known that higher order corrections to the transport equation exist even for low fields, whereas in the discussion above, the application of Eq. (6) does not require the explicit assumption that λ is small nor that we carry out the calculation to the lowest order in λ. The resolution of this apparent paradox lies in the recognition that for any particular distribution of scatterers, the matrix elements of $\hat{\rho}$ are implicit functions of the positions occupied by the scatterers just as in ordinary quantum mechanics, so that the scattered wave is correlated with the position of the scatterer. Thus, when we treat the ensemble average of the product of scattering terms and matrix elements of $\hat{\rho}$ as the product of the ensemble average of the scattering terms multiplied by the ensemble average of the matrix elements of $\hat{\rho}$, we are neglecting this correlation, which would lead to higher order corrections to our equations.

The most obvious example of this correlation effect arises if we consider the diagonal elements of the Liouville equation given by the original Eq. (1) for free electrons interacting with elastic scatterers in the absence of an inhomogeneous field. Then, employing plane waves, which are instantaneous eigenfunctions of $\hat{H}$, we obtain

$$i\hbar \frac{\partial \rho_{\boldsymbol{K}\boldsymbol{K}}}{\partial t} = \sum_{\boldsymbol{K}'} \left(H'_{\boldsymbol{K}\boldsymbol{K}'} \rho_{\boldsymbol{K}'\boldsymbol{K}} - \rho_{\boldsymbol{K}\boldsymbol{K}'} H'_{\boldsymbol{K}'\boldsymbol{K}} \right). \tag{8}$$

Taking the ensemble average of Eq. (8), neglecting the correlation between $\hat{\rho}$ and $\hat{H}'$, and using the fact that for $\boldsymbol{K} \neq \boldsymbol{K}'$, $\hat{H}'$ is a sum of rapidly oscillating terms so $\langle H'_{\boldsymbol{K}\boldsymbol{K}'} \rangle = 0$, we obtain simply $\partial \rho_{\boldsymbol{K}\boldsymbol{K}} / \partial t = 0$. This is, of course, correct only to $O(\lambda)$; the terms of $O(\lambda^2)$, which are the lowest nonvanishing contribution to the scattering rate, have been eliminated by neglecting the correlation between $\hat{\rho}$ and $\hat{H}$.

This discussion also makes it clear why taking the ensemble average of the diagonal elements of Eq. (6) and neglecting correlation between $\hat{\rho}$ and $\hat{H}'$ leads to the correct QTE to $O(\lambda^2)$, whereas doing the same procedure with Eq. (1) does not, because Eq. (6) has scattering terms which are quadratic in $\hat{H}'$ [as mentioned above, the matrix elements of the term involving $\hat{\rho}(t_0)$ is zero if $\rho_{\boldsymbol{K}\boldsymbol{K}'}(t_0)$ is diagonal].

In the next section we will employ Eq. (6) to obtain the equation satisfied by the Wigner function. We will neglect the correlation between matrix elements of $\hat{H}'$ and $\hat{\rho}$, making our results valid through $O(\lambda^2)$.

III. EQUATION FOR WIGNER DISTRIBUTION FUNCTION FOR ELECTRON QUASIPARTICLES INTERACTING WITH ELASTIC SCATTERERS

The total Hamiltonian for this problem consists of $\hat{H} + \hat{H}'$ where $\hat{H}'$ is the Hamiltonian for the impurities, and $\hat{H}$ is the single particle Hamiltonian in the absence of scatterers given by

$$\hat{H} = \mathcal{E}(-i\nabla + \boldsymbol{p}_c/\hbar) + V(\boldsymbol{r}, t), \tag{9}$$

where $\mathcal{E}(\boldsymbol{K})$ is the effective energy band function describing the electron quasiparticle, and

$$\boldsymbol{p}_c(t) \equiv \hbar \boldsymbol{k}_c(t) = \int_{t_0}^{t} dt' e\boldsymbol{E}(t') \tag{10}$$

is the classical momentum acquired by the charged particle due to the the uniform field $\boldsymbol{E}$ turned on at time t_0. Also, $V(\boldsymbol{r},t)$ is an external inhomogeneous potential which is assumed to be time dependent. For the effective single band Hamiltonian

$$\hat{H}_{\mathcal{E}} = \mathcal{E}(-i\nabla + \boldsymbol{k}_c), \tag{11}$$

we take as our basis, the instantaneous eigenfunctions of Eq. (11), given by

$$\psi_{\boldsymbol{K}} = \Omega^{-1/2} e^{i\boldsymbol{K}\boldsymbol{r}}, \tag{12}$$

with the corresponding instantaneous eigenvalues

$$\mathcal{E}(\boldsymbol{K} + \boldsymbol{k}_c) \equiv \mathcal{E}(\boldsymbol{k}); \tag{13}$$

here

$$\boldsymbol{k}(\boldsymbol{K},t) = \boldsymbol{K} + \boldsymbol{k}_c(t), \tag{14}$$

with $\boldsymbol{K}$ satisfying periodic boundary conditions. Consequently, it follows from Eqs. (10) and (11) that $\hbar\boldsymbol{k}$ is the time-dependent quasimomentum of an electron accelerated by the homogeneous field $\boldsymbol{E}(t)$, i.e., $\hbar\dot{\boldsymbol{k}} = \dot{\boldsymbol{p}}_c$, the well known acceleration theorem.

We define the single particle time-dependent Wigner distribution function as

$$F(\boldsymbol{r},\boldsymbol{K},t) \equiv \Omega^{-1} \sum_{\boldsymbol{u}} \rho_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}(t) e^{i\mathbf{u}\mathbf{r}}, \tag{15}$$

where basis states of $\hat{\rho}$ are $\psi_{\boldsymbol{K}}$, given by Eq. (12).

It then follows from Eq. (15) that integrating F over the volume Ω yields the fractional occupancy in state $\boldsymbol{K}$, i.e.,

$$\int_{\Omega} d\boldsymbol{r}\, F(\boldsymbol{r},\boldsymbol{K}) = \rho_{\boldsymbol{K}\boldsymbol{K}}. \tag{16}$$

In addition, it follows from

$$\rho(r) = \mathrm{Tr}\{\hat{\rho}\delta(\boldsymbol{r} - \boldsymbol{r}')\} \tag{17}$$

that the electron density may be calculated from F by

$$\sum_{\boldsymbol{K}} F(\boldsymbol{r},\boldsymbol{K}) = \rho(\boldsymbol{r}). \tag{18}$$

Furthermore, it follows from the Hermiticity of $\hat{\rho}$ that F defined by Eq. (15) is real. Thus, from the sum rules in Eqs. (16) and (18) above, F is viewed as the quantum analog of the Boltzmann distribution function. However, unlike the Boltzmann distribution function, F may take on negative values, so it is not possible to directly associate it with a simultaneous probability distribution in both $\boldsymbol{r}$ and $\boldsymbol{K}$ space.

We can obtain the inverse of Eq. (15) by multiplying both sides by $e^{-i\boldsymbol{u}'\boldsymbol{r}}$ and integrating over the volume Ω. Then, setting $\boldsymbol{u}' = \boldsymbol{K} - \boldsymbol{K}'$, we find

$$\rho_{\boldsymbol{K}\boldsymbol{K}'} = \int_{\Omega} d\boldsymbol{r}\, F\left(\boldsymbol{r}, \frac{\boldsymbol{K}+\boldsymbol{K}'}{2}\right) e^{-i(\boldsymbol{K}-\boldsymbol{K}')\boldsymbol{r}}. \tag{19}$$

Thus, in utilizing Eq. (19), any equation satisfied by the matrix elements of $\hat{\rho}$ can be transformed into an (integral) equation for F.

In general, the expectation value for any arbitrary operator $\hat{B}$ can be evaluated as

$$\langle B \rangle = \mathrm{Tr}\{\hat{\rho}\hat{B}\} \equiv \sum_{\boldsymbol{K}} \int_{\Omega} d\boldsymbol{r}\, F(\boldsymbol{r},\boldsymbol{K}) B_W(\boldsymbol{r},\boldsymbol{K}), \tag{20}$$

where B_W is a Wigner-Weyl form of the operator, given by

$$B_W(\boldsymbol{r},\boldsymbol{K}) \equiv \Omega^{-1} \sum_{\boldsymbol{u}} B_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}(t) e^{i\boldsymbol{u}\boldsymbol{r}}.$$

For the particular case of the local coordinate-dependent operator $B(\boldsymbol{r})$, the equation for $\langle B \rangle$ further reduces to

$$\langle B \rangle = \sum_{\boldsymbol{K}} \int_{\Omega} d\boldsymbol{r}\, F(\boldsymbol{r},\boldsymbol{K}) B(\boldsymbol{r}).$$

Alternatively, if the operator $\hat{B}$ is diagonal in the $\boldsymbol{K}$ basis, i.e., $B_{\boldsymbol{K}\boldsymbol{K}'} = B_{\boldsymbol{K}}\delta_{\boldsymbol{K}\boldsymbol{K}'}$, then

$$\langle B \rangle = \sum_{\boldsymbol{K}} \int_{\Omega} d\boldsymbol{r}\, F(\boldsymbol{r},\boldsymbol{K}) B_{\boldsymbol{K}};$$

such is the case for the velocity operator associated with the quasiparticle electron system described by Eq. (9) where

$$\boldsymbol{v}_{\boldsymbol{K}\boldsymbol{K}'} = \boldsymbol{v}_{\boldsymbol{K}}\delta_{\boldsymbol{K}\boldsymbol{K}'}, \quad \text{with } \boldsymbol{v}_{\boldsymbol{K}} = \hbar^{-1}\nabla_{\boldsymbol{K}}\mathcal{E}(\boldsymbol{K} + \boldsymbol{k}_c). \tag{21}$$

Note that in general F and B_W are basis dependent, whereas expectation values are basis independent.

Now we proceed to derive the Wigner transform of the Liouville equation given by Eq. (6). Taking the $\boldsymbol{K}+\boldsymbol{u}/2$, $\boldsymbol{K}-\boldsymbol{u}/2$ matrix elements of Eq. (6), multiplying both sides of the resulting equation by $e^{i\boldsymbol{u}\boldsymbol{r}}/\Omega$, summing over $\boldsymbol{u}$ and dividing by $i\hbar$ yields

$$\frac{\partial F}{\partial t} = T_{\mathcal{E}} + T_V + C^{(1)} + C^{(2)}, \tag{22}$$

where

$$T_{\mathcal{E}} = -\frac{i}{\hbar\Omega} \sum_{\boldsymbol{u}} \left\{ \mathcal{E}\left(\boldsymbol{k} + \frac{\boldsymbol{u}}{2}\right) - \mathcal{E}\left(\boldsymbol{k} - \frac{\boldsymbol{u}}{2}\right) \right\} \rho_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2} e^{i\boldsymbol{u}\boldsymbol{r}}, \tag{23}$$

$$T_V = -\frac{i}{\hbar\Omega} \sum_{\boldsymbol{u}} [V, \hat{\rho}]_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2} e^{i\boldsymbol{u}\boldsymbol{r}}, \tag{24}$$

and $C^{(1)}$, $C^{(2)}$ are derived from the linear-in-$\hat{H}'$ and quadratic-in-$\hat{H}'$ terms on the right-hand side of Eq. (6), respectively.

We note first that for parabolic dispersion, the $T_{\mathcal{E}}$ term is simply related to the usual diffusion term, since in this case, with $\mathcal{E}(\boldsymbol{k}) = \hbar^2\boldsymbol{k}^2/2m$, we have the exact relation

$$\mathcal{E}\left(\boldsymbol{k}+\frac{\boldsymbol{u}}{2}\right)-\mathcal{E}\left(\boldsymbol{k}-\frac{\boldsymbol{u}}{2}\right)=\nabla_{\boldsymbol{K}}\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)\boldsymbol{u}, \tag{25}$$

which results in

$$T_{\mathcal{E}}=-\hbar^{-1}\nabla_{\boldsymbol{K}}\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)\nabla_{\boldsymbol{r}}F. \tag{26}$$

Equation (26) is the usual diffusion term as found in the BTE provided we neglect the implicit field dependence given by $\boldsymbol{k}_c$.

More generally, for arbitrarily dispersion we have

$$T_{\mathcal{E}}=-\frac{i}{\hbar}\sum_{\boldsymbol{u}}\left\{\mathcal{E}\left(\boldsymbol{k}+\frac{\boldsymbol{u}}{2}\right)-\mathcal{E}\left(\boldsymbol{k}-\frac{\boldsymbol{u}}{2}\right)\right\}\times\int_{\Omega}d\boldsymbol{r}'\,F(\boldsymbol{r}',\boldsymbol{K})e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')}, \tag{27}$$

where we have used Eq. (19) to write $T_{\mathcal{E}}$ in terms of F in its integral form. Alternatively, $T_{\mathcal{E}}$ may be presented in a differential form by expanding the energy difference in Eq. (23) about $\boldsymbol{u}=0$ and then summing all the terms. This is facilitated by noting that

$$\mathcal{E}\left(\boldsymbol{k}+\frac{\boldsymbol{u}}{2}\right)e^{i\boldsymbol{u}\boldsymbol{r}}=e^{\nabla_{\boldsymbol{K}}\cdot(\boldsymbol{u}/2)}\{\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)e^{i\boldsymbol{u}\boldsymbol{r}}\}=e^{-(i/2)\nabla_{\boldsymbol{K}}\cdot\nabla_{\boldsymbol{r}}}\{\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)e^{i\boldsymbol{u}\boldsymbol{r}}\}, \tag{28}$$

so

$$T_{\mathcal{E}}=-\frac{i}{\hbar\Omega}(e^{-(i/2)\nabla_{\boldsymbol{K}}\cdot\nabla_{\boldsymbol{r}}}-e^{(i/2)\nabla_{\boldsymbol{K}}\cdot\nabla_{\boldsymbol{r}}})\times\left\{\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)\sum_{\boldsymbol{u}}\rho_{\boldsymbol{K}'+\boldsymbol{u}/2,\boldsymbol{K}'-\boldsymbol{u}/2}e^{i\boldsymbol{u}\boldsymbol{r}}\right\}_{\boldsymbol{K}'=\boldsymbol{K}}. \tag{29}$$

Then using Eq. (15), we obtain

$$T_{\mathcal{E}}=-2\hbar^{-1}\sin(\nabla_{\boldsymbol{K}}\cdot\nabla_{\boldsymbol{r}}/2)\{\mathcal{E}(\boldsymbol{K}+\boldsymbol{k}_c)F(\boldsymbol{r},\boldsymbol{K}')\}_{\boldsymbol{K}'=\boldsymbol{K}}, \tag{30}$$

which obviously reduces to Eq. (26) if only the first term in the expansion is retained. Thus, we obtain again the usual diffusion term in the limit of parabolic dispersion; there are additional terms contained in Eq. (30) for a more general energy dispersion which are not found in the BTE, in agreement with the results of Charbonneau *et al.*[13]

Similarly, the T_V term in Eq. (24) may be rewritten as

$$T_V=-\frac{i}{\hbar\Omega}\sum_{\boldsymbol{u},\boldsymbol{K}'}(V_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'+\boldsymbol{u}/2}\rho_{\boldsymbol{K}'+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}-\rho_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'-\boldsymbol{u}/2}V_{\boldsymbol{K}'-\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2})e^{i\boldsymbol{u}\boldsymbol{r}}. \tag{31}$$

Then using Eq. (19), and the fact that $V(\boldsymbol{r},t)$ is a local operator so

$$V_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'+\boldsymbol{u}/2}=\frac{1}{\Omega}\int_{\Omega}d\boldsymbol{r}\,V(\boldsymbol{r})e^{-i(\boldsymbol{K}-\boldsymbol{K}')\boldsymbol{r}}\equiv V_{\boldsymbol{K}-\boldsymbol{K}'}, \tag{32}$$

independent of $\boldsymbol{u}$, we obtain, without approximation

$$T_V=-\frac{i}{\hbar}\sum_{\boldsymbol{q}}V_{\boldsymbol{q}}e^{i\boldsymbol{q}\boldsymbol{r}}\left\{F\left(\boldsymbol{r},\boldsymbol{K}-\frac{\boldsymbol{q}}{2}\right)-F\left(\boldsymbol{r},\boldsymbol{K}+\frac{\boldsymbol{q}}{2}\right)\right\}. \tag{33}$$

If the potential is slowly varying in space, then $V_{\boldsymbol{q}}$ is significant only for small $\boldsymbol{q}$. Then expanding F in Eq. (33) about $\boldsymbol{q}=0$ and retaining only the lowest nonzero term we obtain

$$T_V\approx\hbar^{-1}\nabla_{\boldsymbol{r}}V\cdot\nabla_{\boldsymbol{K}}F=-\hbar^{-1}e\boldsymbol{E}_V\cdot\nabla_{\boldsymbol{K}}F, \tag{34}$$

where $e\boldsymbol{E}_V(\boldsymbol{r},t)=-\nabla_{\boldsymbol{r}}V$ defines the electric field corresponding to the inhomogeneous potential energy V. Thus, this term accounts for the contribution of the inhomogeneous part of the electric field to the usual drift term in Eq. (22). Had we taken our basis functions as eigenfunctions of a Hamiltonian in which $\boldsymbol{k}_c\equiv 0$ for all t, V would be the total potential arising from both the applied and inhomogeneous potentials. In such a case the $\boldsymbol{E}_V$ in Eq. (34) would be the total position-dependent electric field. We will show below that choosing a vector potential gauge in which $\boldsymbol{k}_c\neq 0$ also leads to the same total drift term and simultaneously enables us to include high field effects in the collision term.[9] T_V may be transformed from its integral form as given by Eq. (33) to a differential form by expanding F about $\boldsymbol{q}=0$ and summing all the terms. Using similar arguments as those that led from Eq. (27) to Eq. (29) we readily obtain the so-called Moyal[21] expansion

$$T_V=2\hbar^{-1}\sin(\nabla_{\boldsymbol{K}}\cdot\nabla_{\boldsymbol{r}}/2)\{V(\boldsymbol{r})F(\boldsymbol{r}',\boldsymbol{K})\}_{\boldsymbol{r}'=\boldsymbol{r}}, \tag{35}$$

the first term in the expression of Eq. (35) being the approximation given by Eq. (34). Charbonneau *et al.*[13] do not obtain a term like that given by Eq. (33) because they do not include the effect of an inhomogeneous field. However, a similar term was found by Wigner[10] and discussed by Iafrate *et al.*[11] with respect to its effect in transport theory. Equation (31) is the generalization of a result of Price[12] who considered a perturbation consisting of a single Fourier component in wavelength and frequency.

Thus far our derivations of the generalized drift term as given by Eq. (27) or (30) and the generalized diffusion term as given by Eq. (33) or (35) are exact so that in the absence of any scattering term, the equation for the Wigner distribution function is exact for arbitrary strength and time dependence of both the homogeneous field given by the vector potential and the inhomogeneous field given by V.

We now consider the evaluation of the two collision terms in Eq. (22), one linear in the scattering potential $\hat{H}'$ involving the density operator at time $t=t_0$ and the second quadratic in $\hat{H}'$. We consider the quadratic term first. We observe that the Hamiltonian that appears in $\hat{U}$ of Eq. (3) is given by Eq. (9) and includes the inhomogeneous potential V; this makes the matrix elements which depend explicitly upon $\hat{U}$, namely, $C^{(1)}$ and $C^{(2)}$, in Eq. (22) difficult to evaluate since the basis states employed are the instantaneous eigenfunctions of the Hamiltonian given by Eq. (11) which exclude V. However, we proceed to show the relationship between $\hat{U}$ and V, and then to approximate $\hat{U}$ matrix elements for the purpose of calculating $C^{(2)}$ and $C^{(1)}$.

In a fashion similar to the derivation of Eq. (6), let us express the time evolution operator $\hat{U}$ corresponding to the

Hamiltonian $\hat{H}=\hat{H}_0+V$ in terms of the time evolution operator $\hat{U}_0$ corresponding to $\hat{H}_0$. Integrating $i\hbar\partial(\hat{U}_0^+\hat{U})/\partial t$, and using $i\hbar\partial\hat{U}_0/\partial t=\hat{H}_0\hat{U}_0$ and $i\hbar\partial\hat{U}/\partial t=\hat{H}\hat{U}$, we solve for $\hat{U}$ to obtain an exact integral equation for $\hat{U}$ as

$$\hat{U}(t,t_0)=\hat{U}_0(t,t_0)\left\{\hat{\mathbb{1}}-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{U}_0(t_0,t')V(t')\hat{U}(t',t_0)\right\}. \tag{36}$$

Then substituting $\hat{U}_0$ for $\hat{U}$ under the integral results in the approximate first-order-in-V closed equation for the operator $\hat{U}$. Evaluating matrix elements of this operator results in

$$U_{\boldsymbol{K}\boldsymbol{K}'}(t,t_0)\approx e^{-(i/\hbar)\int_{t_0}^{t}dt'\,\mathcal{E}(\boldsymbol{k})}\left[\delta_{\boldsymbol{K}\boldsymbol{K}'}-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,V_{\boldsymbol{K}-\boldsymbol{K}'}(t')\times e^{(i/\hbar)\int_{t_0}^{t'}dt''\{\mathcal{E}(\boldsymbol{k})-\mathcal{E}(\boldsymbol{k}')\}}\right]. \tag{37}$$

Note that everywhere else we are going to use an abbreviation for the *action* (normalized to $\hbar$)

$$s_{\boldsymbol{k}}(t,t_0)=-\hbar^{-1}\int_{t_0}^{t}dt'\,\mathcal{E}(\boldsymbol{k}). \tag{38}$$

Equation (37) allows us to go beyond $O(\lambda^2\lambda_V^0)$ in approximating $C^{(2)}$ with increased analytical complexity (here λ_V is the strength of the inhomogeneous potential V and λ is the strength of the scattering interaction, as mentioned earlier).

However, it is clear from Eq. (37) that the off-diagonal term due to the scattering from the inhomogeneous potential includes collision broadening that becomes quite pronounced for conditions of strong electric fields and for situations involving large momentum transfer. If the inhomogeneous potential V is treated as slowly varying, then momentum transfer processes and the corresponding broadening effects are small; thus the effect of V in $C^{(2)}$ is heavily masked by the strong large-angle impurity scattering. Therefore, since we are specifically interested in the limit of slowly varying inhomogeneous potential, we retain only the first term in Eq. (37) so that the term quadratic in $\hat{H}'$ is (formally) evaluated only to $O(\lambda^2\lambda_V^0)$. We will, of course, continue to treat the strength and time dependence of the homogeneous field as unrestricted.[22]

Then from Eq. (6) the term quadratic in $\hat{H}'$ appearing in Eq. (22) may be written

$$C^{(2)}=-\frac{1}{\hbar^2\Omega}\sum_{\boldsymbol{u}}\left[\hat{H}'(t),\int_{t_0}^{t}dt'\,\hat{U}(t,t')\times[\hat{H}'(t'),\hat{\rho}(t')]\hat{U}(t',t)\right]_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}e^{i\boldsymbol{u}\boldsymbol{r}}. \tag{39}$$

Expanding the commutator, inserting complete sets of states, and keeping only the first term in Eq. (37), i.e.,

$$U_{\boldsymbol{K}\boldsymbol{K}'}(t,t_0)\approx e^{is_{\boldsymbol{k}}(t,t_0)}\delta_{\boldsymbol{K}\boldsymbol{K}'}, \tag{40}$$

$C^{(2)}$ can be written as a sum of two terms, in the form $C^{(2)}=C_1^{(2)}+C_2^{(2)}$. Here,

$$C_1^{(2)}=-\frac{1}{\hbar^2\Omega}\sum_{\boldsymbol{u},\boldsymbol{K}'}H'_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'+\boldsymbol{u}/2}(t)\times\int_{t_0}^{t}dt'[\hat{H}'(t'),\hat{\rho}(t')]_{\boldsymbol{K}'+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}\times e^{i\{s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t')-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t')\}}e^{i\boldsymbol{u}\boldsymbol{r}}. \tag{41}$$

Similarly, we find that the other term $C_2^{(2)}$ obtained from the commutator in Eq. (39) satisfies $C_2^{(2)}=C_1^{(2)*}$ so $C^{(2)}$ is actually real and equal to $2\,\mathrm{Re}\,C_1^{(2)}$.

Now, like Eq. (32), for the basis states involved, we find that

$$H'_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'+\boldsymbol{u}/2}=\Omega^{-1}\int_{\Omega}d\boldsymbol{r}\,\hat{H}'e^{-i(\boldsymbol{K}-\boldsymbol{K}')\boldsymbol{r}}\equiv H'_{\boldsymbol{K}-\boldsymbol{K}'}. \tag{42}$$

Then, in evaluating the matrix elements of the commutator in Eq. (41), by inserting complete sets of states, we have, using Eq. (42)

$$C_1^{(2)}=-\frac{1}{\hbar^2\Omega}\sum_{\boldsymbol{u},\boldsymbol{K}',\boldsymbol{K}''}H'_{\boldsymbol{K}-\boldsymbol{K}'}(t)\int_{t_0}^{t}dt'\{H'_{\boldsymbol{K}'-\boldsymbol{K}''}(t')\rho_{\boldsymbol{K}''+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}-\rho_{\boldsymbol{K}'+\boldsymbol{u}/2,\boldsymbol{K}''-\boldsymbol{u}/2}H'_{\boldsymbol{K}''-\boldsymbol{K}}(t')\}e^{i\{s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t')-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t')\}}e^{i\boldsymbol{u}\boldsymbol{r}}. \tag{43}$$

Using Eq. (19) we may write Eq. (43) as

$$C_1^{(2)}=-\frac{1}{\hbar^2\Omega}\sum_{\boldsymbol{u},\boldsymbol{K}',\boldsymbol{K}''}H'_{\boldsymbol{K}-\boldsymbol{K}'}(t)\int_{t_0}^{t}dt'\left\{H'_{\boldsymbol{K}'-\boldsymbol{K}''}(t')\int_{\Omega}d\boldsymbol{r}'F\left(\boldsymbol{r}',\frac{\boldsymbol{K}''+\boldsymbol{K}}{2},t'\right)e^{-i(\boldsymbol{K}''-\boldsymbol{K})\boldsymbol{r}'}e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')}-H'_{\boldsymbol{K}''-\boldsymbol{K}}(t')\int_{\Omega}d\boldsymbol{r}'F\left(\boldsymbol{r}',\frac{\boldsymbol{K}'+\boldsymbol{K}''}{2},t'\right)e^{-i(\boldsymbol{K}'-\boldsymbol{K}'')\boldsymbol{r}'}e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')}\right\}e^{i\{s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t')-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t')\}}. \tag{44}$$

Now, as already discussed in Sec. II, $\hat{\rho}$ (and consequently F) implicitly depends on the exact location of the scatterers. If we take the ensemble average of Eq. (22) over the distribution of scatterers, we can replace $\hat{\rho}$ and F by their ensemble averages (which we will continue to denote by $\hat{\rho}$ and F, respectively, without ambiguity) without approximation in all terms other than the scattering terms because the operators acting on them are uncorrelated with the microscopic distribution of the scatterers. In order to calculate the ensemble average of the term involving the product of matrix elements of $\hat{H}'$ and F, we will neglect the correlation so that our results will be valid through $O(\lambda^2)$.

Now if the impurities are located at sites $\boldsymbol{r}_i$, with $i=1,\ldots,N$, then

$$\hat{H}'(t)=\sum_{i=1}^{N}\phi(\boldsymbol{r}-\boldsymbol{r}_i,t), \tag{45}$$

where we have allowed for the possibility of time-dependent screening. Then

$$H'_{\boldsymbol{K}}(t)H'_{-\boldsymbol{K}+\boldsymbol{q}}(t')=\phi_{\boldsymbol{K}}(t)\phi_{-\boldsymbol{K}+\boldsymbol{q}}(t')\sum_{i,j}e^{-i\boldsymbol{K}(\boldsymbol{r}_i-\boldsymbol{r}_j)}e^{-i\boldsymbol{q}\boldsymbol{r}_j}, \tag{46}$$

where

$$\phi_{\boldsymbol{K}}=\int_{\Omega}d\boldsymbol{r}\;\phi(\boldsymbol{r})e^{-i\boldsymbol{K}\boldsymbol{r}}. \tag{47}$$

If we assume that the $\{\boldsymbol{r}_i\}$ are randomly (although not necessarily homogeneously) distributed, then the major contribution to the sum in Eq. (46) comes from the terms $i=j$, in which case we will replace the product of the matrix elements of $\hat{H}'$ by

$$\langle H'_{\boldsymbol{K}}(t)H'_{-\boldsymbol{K}+\boldsymbol{q}}(t')\rangle=\phi_{\boldsymbol{K}}(t)\phi_{-\boldsymbol{K}+\boldsymbol{q}}(t')\left\langle\sum_j e^{-i\boldsymbol{q}\boldsymbol{r}_j}\right\rangle. \tag{48}$$

If $n(\boldsymbol{r})$ is the average density of scatterers at point $\boldsymbol{r}$ then

$$\left\langle\sum_j e^{-i\boldsymbol{q}\boldsymbol{r}_j}\right\rangle=\int_{\Omega}d\boldsymbol{r}\;n(\boldsymbol{r})e^{-i\boldsymbol{q}\boldsymbol{r}}\equiv n_{\boldsymbol{q}}, \tag{49}$$

so that

$$\langle H'_{\boldsymbol{K}}(t)H'_{-\boldsymbol{K}+\boldsymbol{q}}(t')\rangle=n_{\boldsymbol{q}}\phi_{\boldsymbol{K}}(t)\phi_{-\boldsymbol{K}+\boldsymbol{q}}(t'). \tag{50}$$

For a homogeneous distribution of scatterers $n_{\boldsymbol{q}}=(N/\Omega)\delta_{\boldsymbol{q},0}$, so Eq. (50) agrees with Eq. (7) for $\boldsymbol{q}\neq 0$ and agrees with the usual result[2] for $\boldsymbol{q}=0$.

Then substituting Eq. (50) into the ensemble averaged Eq. (44) and using the fact that $C^{(2)}=2\,\mathrm{Re}\,C_1^{(2)}$, we obtain, for the quadratic-in-$\hat{H}'$ collision term, to $O(\lambda^2)$

$$C^{(2)}=\frac{2}{\hbar^2\Omega}\mathrm{Re}\sum_{\boldsymbol{u},\boldsymbol{K}',\boldsymbol{q}}n_{\boldsymbol{q}}\phi_{\boldsymbol{K}-\boldsymbol{K}'}(t)\int_{t_0}^{t}dt'\,\phi_{\boldsymbol{K}'-\boldsymbol{K}+\boldsymbol{q}}(t')\times e^{i\{s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t')-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t')\}}\times\int_{\Omega}d\boldsymbol{r}'\left\{F\left(\boldsymbol{r}',\boldsymbol{K}'+\frac{\boldsymbol{q}}{2},t'\right)-F\left(\boldsymbol{r}',\boldsymbol{K}-\frac{\boldsymbol{q}}{2},t'\right)\right\}$$
$$\times e^{i\boldsymbol{q}\boldsymbol{r}'}e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')}. \tag{51}$$

Finally, from Eq. (6) the term linear in $\hat{H}'$ appearing in Eq. (22) is

$$C^{(1)}=-\frac{i}{\hbar\Omega}\sum_{\boldsymbol{u}}[\hat{H}'(t),\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}(t_0,t)]_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}e^{i\boldsymbol{u}\boldsymbol{r}}. \tag{52}$$

Then neglecting the inhomogeneous potential V in $\hat{H}$ as in the evaluation of $C^{(2)}$, and inserting a complete set of states, we find

$$C^{(1)}=-\frac{i}{\hbar\Omega}\sum_{\boldsymbol{u},\boldsymbol{K}'}\{H'_{\boldsymbol{K}-\boldsymbol{K}'}(t)\rho_{\boldsymbol{K}'+\boldsymbol{u}/2,\boldsymbol{K}-\boldsymbol{u}/2}(t_0)\times e^{i[s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t_0)-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t_0)]}-\rho_{\boldsymbol{K}+\boldsymbol{u}/2,\boldsymbol{K}'-\boldsymbol{u}/2}(t_0)H'_{\boldsymbol{K}'-\boldsymbol{K}}(t)e^{i[s_{\boldsymbol{k}+\boldsymbol{u}/2}(t,t_0)-s_{\boldsymbol{k}'-\boldsymbol{u}/2}(t,t_0)]}\}. \tag{53}$$

We observe that $C^{(1)}$ is a memory term[5] depending on the distribution function $\hat{\rho}$ at an initial time t_0. Now if this initial distribution function is uncorrelated with $\hat{H}'$ (as it would be if we injected the electrons at $t=t_0$) then the ensemble average over the scatterers of $C^{(1)}$ is exactly zero because the ensemble average of $\hat{H}'$ is zero, where we have assumed that the (independent of $\boldsymbol{K}$) diagonal elements, $H'_{\boldsymbol{K}\boldsymbol{K}}=N\phi_0=\mathrm{const}$, have been absorbed into the energy dispersion $\mathcal{E}(\boldsymbol{K})$. Alternatively, if we assume that the interaction with the scatterers is turned on very slowly so that $\hat{H}'\to 0$ for $t_0\to-\infty$ as done by Levinson[4] for phonon scattering, we have the distribution for $t_0\to-\infty$ completely uncorrelated with the positions of the scatterers with the consequence that the ensemble average of $C^{(1)}$ is again zero. We will therefore consider only the case where

$$C^{(1)}=0; \tag{54}$$

so substituting Eqs. (27), (33), (51), and (54) into Eq. (22) yields the QTE for the Wigner distribution function in the $\boldsymbol{K}$ representation.

As in the case when only a homogeneous field is present we can transform to a new set of variables which result in the more conventional representation.[6,9] We transform from $(\boldsymbol{K},t)$ to $(\boldsymbol{k},t)$ variables by using Eq. (14), and note that $F(\boldsymbol{r},\boldsymbol{K},t)$ becomes $W(\boldsymbol{r},\boldsymbol{k},t)$, that is

$$W(\boldsymbol{r},\boldsymbol{k},t)\equiv F(\boldsymbol{r},\boldsymbol{K},t) \tag{55}$$

is the Wigner function in the $\boldsymbol{k}$ representation.

It follows from Eqs. (14) and (55) that

$$\frac{\partial F}{\partial t}=\frac{\partial W}{\partial t}+\hbar^{-1}e\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}W, \tag{56}$$

where $e\boldsymbol{E}$ is the force on the electron due to the homogeneous field $\boldsymbol{E}$. Also from Eq. (14) it follows that[6]

$$\boldsymbol{k}(\boldsymbol{K},t')=\boldsymbol{k}(\boldsymbol{K},t)-\{\boldsymbol{k}_c(t)-\boldsymbol{k}_c(t')\} \tag{57}$$

and from Eq. (47)

$$\phi_{K-K'} = \phi_{k-k'}. \tag{58}$$

Then in terms of $(\boldsymbol{k},t)$ variables the QTE given by Eq. (22) takes the form

$$\frac{\partial W}{\partial t} + \hbar^{-1} e\boldsymbol{E}(t)\cdot\nabla_{\boldsymbol{k}} W - T_{\mathcal{E}} - T_V = C^{(2)}, \tag{59}$$

where from Eqs. (27) and (33) and Eqs. (30) and (35) the integral and differential forms of $T_{\mathcal{E}}$ and T_V are given by

$$T_{\mathcal{E}} = -i\hbar^{-1}\sum_{\boldsymbol{u}}\left\{\mathcal{E}\left(\boldsymbol{k}+\frac{\boldsymbol{u}}{2}\right)-\mathcal{E}\left(\boldsymbol{k}-\frac{\boldsymbol{u}}{2}\right)\right\}\int_{\Omega} d\boldsymbol{r}'\, W(\boldsymbol{r}',\boldsymbol{k})e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')} \equiv -2\hbar^{-1}\sin(\nabla_{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{r}}/2)\{\mathcal{E}(\boldsymbol{k})W(\boldsymbol{r},\boldsymbol{k}')\}_{\boldsymbol{k}'=\boldsymbol{k}}, \tag{60}$$

$$T_V = -i\hbar^{-1}\sum_{\boldsymbol{q}} V_{\boldsymbol{q}} e^{i\boldsymbol{q}\boldsymbol{r}}\left\{W\left(\boldsymbol{r},\boldsymbol{k}-\frac{\boldsymbol{q}}{2}\right)-W\left(\boldsymbol{r},\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\right)\right\} \equiv 2\hbar^{-1}\sin(\nabla_{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{r}}/2)\{V(\boldsymbol{r})W(\boldsymbol{r}',\boldsymbol{k})\}_{\boldsymbol{r}'=\boldsymbol{r}}, \tag{61}$$

and from Eq. (51)

$$C^{(2)} = \frac{2}{\hbar^2\Omega}\mathrm{Re}\sum_{\boldsymbol{u},\boldsymbol{k}',\boldsymbol{q}} n_{\boldsymbol{q}}\phi_{\boldsymbol{k}-\boldsymbol{k}'}(t)\int_{t_0}^{t} dt'\,\phi_{\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}}(t')e^{i\{s_{\boldsymbol{k}'+\boldsymbol{u}/2}(t,t')-s_{\boldsymbol{k}-\boldsymbol{u}/2}(t,t')\}}\int_{\Omega} d\boldsymbol{r}'\left\{W\left(\boldsymbol{r}',\boldsymbol{k}'+\frac{\boldsymbol{q}}{2},t'\right)-W\left(\boldsymbol{r}',\boldsymbol{k}-\frac{\boldsymbol{q}}{2},t'\right)\right\}e^{i\boldsymbol{q}\boldsymbol{r}'}e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}')}. \tag{62}$$

Thus, given that the Wigner function $W(\boldsymbol{r},\boldsymbol{k},t)$ in Eq. (59) is in the $\boldsymbol{k}$ representation, it then follows that observables like the velocity can be calculated as

$$\langle\boldsymbol{v}\rangle = \sum_{\boldsymbol{k}}\int_{\Omega} d\boldsymbol{r}\, W(\boldsymbol{r},\boldsymbol{k})\boldsymbol{v}_{\boldsymbol{k}}, \tag{63}$$

where $\boldsymbol{v}_{\boldsymbol{k}} = \hbar^{-1}\nabla_{\boldsymbol{k}}\mathcal{E}(\boldsymbol{k})$.

IV. DISCUSSION OF RESULTS

Equation (59), the QTE for the Wigner distribution function, was derived by neglecting the effect of the inhomogeneous potential on the scattering, but treating the generalization of the drift and diffusion terms exactly. In the limit in which there is no inhomogeneous potential and the impurity distribution is random and homogeneous, W will be independent of $\boldsymbol{r}$. In this case, $T_{\mathcal{E}}=T_V=0$ and the integral over $\boldsymbol{r}'$ in $C^{(2)}$ can be done which yields a term $\sim\delta_{\boldsymbol{u},\boldsymbol{q}}$. When the sum over $\boldsymbol{u}$ is performed as well as the one over $\boldsymbol{q}$ using $n_{\boldsymbol{q}} = (N/\Omega)\delta_{\boldsymbol{q},0}$ for a homogeneous distribution of scatterers, we obtain the equation previously derived for the homogeneous case[9] including the intracollisional field effect in the scattering term.[4,5]

In the limit when V is slowly varying we can approximate $T_{\mathcal{E}}$ and T_V by the first terms in the expansions given by Eqs. (60) and (61) in which case Eq. (59) becomes readily

$$\frac{\partial W}{\partial t} + \hbar^{-1} e\boldsymbol{E}_{\mathrm{total}}\cdot\nabla_{\boldsymbol{k}} W + \boldsymbol{v}_{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{r}} W = C^{(2)}, \tag{64}$$

where $e\boldsymbol{E}_{\mathrm{total}}(\boldsymbol{r},t) = e\boldsymbol{E}(t) + e\boldsymbol{E}_V(\boldsymbol{r},t)$ is the total position and time-dependent force acting on the electron.

The left-hand side (lhs) of Eq. (64) repeats exactly the lhs of the BTE but has been derived directly from the Liouville equation for $\boldsymbol{E}_{\mathrm{total}}$ of arbitrary strength and time dependence, with the only approximation being that V is slowly varying over space. If in addition we assume that the density of scatterers is slowly varying over a wavelength of a typical electron, then $n_{\boldsymbol{q}}$ is large only for $\boldsymbol{q}$ small compared to the typical $\boldsymbol{k}$. Then neglecting the $\boldsymbol{q}$ dependence of the matrix elements $\phi_{\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}}$ and also in W, summing the remaining terms over $\boldsymbol{q}$, we find the integrand for $C^{(2)}$ is $n(\boldsymbol{r}')$, so the local density of scatterers is multiplied by matrix elements of ϕ similar to that given by the golden rule of time-dependent perturbation theory. If we further assume that $n(\boldsymbol{r}')W(\boldsymbol{r}',\boldsymbol{k},t)$ is slowly varying with respect to $\boldsymbol{r}'$, then we may evaluate it in the integral over $\boldsymbol{r}'$ at $\boldsymbol{r}=\boldsymbol{r}'$ since it is multiplied by a rapidly varying function peaked at this point. Then the integral over $\boldsymbol{r}'$ may be performed yielding a term $\sim\delta_{\boldsymbol{u},0}$. Then summing over $\boldsymbol{u}$ and neglecting the possibility of time-dependent screening, we obtain

$$C^{(2)} = \frac{2}{\hbar^2}n(\boldsymbol{r})\sum_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}-\boldsymbol{k}'}|^2\int_{t_0}^{t} dt'\{W(\boldsymbol{r},\boldsymbol{k}',t') - W(\boldsymbol{r},\boldsymbol{k},t')\}\cos\{s_{\boldsymbol{k}'}(t,t') - s_{\boldsymbol{k}}(t,t')\}, \tag{65}$$

which is the generalization of the Boltzmann scattering term that accounts for the intracollisional field effect. If the field dependence is neglected in Eq. (65), then $C^{(2)}$ may be shown to be equivalent to the scattering term in the usual BTE by making an expansion of Eq. (65) as previously done for the case of the homogeneous field.[2]

The collision term in a general form given by Eq. (62) is much more complicated than the corresponding result for the

homogeneous case, requiring additional sums over $\boldsymbol{u}$ and $\boldsymbol{q}$ as well as an integral over $\boldsymbol{r}'$. However, for parabolic dispersion the sum over $\boldsymbol{u}$ may be done explicitly, because in this case

$$\mathcal{E}\left(\boldsymbol{k}'+\frac{\boldsymbol{u}}{2}\right)-\mathcal{E}\left(\boldsymbol{k}-\frac{\boldsymbol{u}}{2}\right) = \mathcal{E}(\boldsymbol{k}')-\mathcal{E}(\boldsymbol{k})+\{\nabla_{\boldsymbol{k}'}\mathcal{E}(\boldsymbol{k}')+\nabla_{\boldsymbol{k}}\mathcal{E}(\boldsymbol{k})\}\boldsymbol{u}/2 \tag{66}$$

exactly, for arbitrary $\boldsymbol{u}$, and therefore

$$\frac{1}{\hbar}\int_{t'}^{t} d\tau\{\nabla_{\boldsymbol{k}'}\mathcal{E}(\boldsymbol{k}')+\nabla_{\boldsymbol{k}}\mathcal{E}(\boldsymbol{k})\}\frac{\boldsymbol{u}}{2}=\int_{t'}^{t} d\tau\frac{\boldsymbol{v}_{\boldsymbol{k}'}+\boldsymbol{v}_{\boldsymbol{k}}}{2}\boldsymbol{u} \equiv \bar{\boldsymbol{r}}(\boldsymbol{k},\boldsymbol{k}',t,t')\boldsymbol{u}, \tag{67}$$

where $\bar{\boldsymbol{r}}$ is the displacement of an electron during the interval t' to t as it is being accelerated by the homogeneous field. The $\boldsymbol{u}$ dependent term in Eq. (62) may then be summed using

$$\Omega^{-1}\sum_{\boldsymbol{u}} e^{i\boldsymbol{u}(\boldsymbol{r}-\boldsymbol{r}'-\bar{\boldsymbol{r}})}=\delta(\boldsymbol{r}-\boldsymbol{r}'-\bar{\boldsymbol{r}}). \tag{68}$$

The result for $C^{(2)}$ is then

$$C^{(2)}=\frac{2}{\hbar^2}\mathrm{Re}\sum_{\boldsymbol{k}',\boldsymbol{q}} n_{\boldsymbol{q}}\phi_{\boldsymbol{k}-\boldsymbol{k}'}(t)\int_{t_0}^{t} dt'\,\phi_{\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q}}(t') \times\left\{W\left(\boldsymbol{r}-\bar{\boldsymbol{r}},\boldsymbol{k}'+\frac{\boldsymbol{q}}{2},t'\right)-W\left(\boldsymbol{r}-\bar{\boldsymbol{r}},\boldsymbol{k}'-\frac{\boldsymbol{q}}{2},t'\right)\right\}, \times e^{i\{s_{\boldsymbol{k}'}(t,t')-s_{\boldsymbol{k}}(t,t')\}}e^{i\boldsymbol{q}(\boldsymbol{r}-\bar{\boldsymbol{r}})}, \tag{69}$$

in the parabolic dispersion approximation. Equation (69) is the generalization of a result of Price.[12] Using the same arguments as Price, we conclude that in the weak field limit, $\bar{\boldsymbol{r}}$ is of the order of a typical de Broglie wavelength so that its appearance in Eq. (69) will be significant only if W changes appreciably over such dimensions, i.e., V or n vary significantly over a de Broglie wavelength.

V. SUMMARY

The quantum transport equation for a Bloch electron in a single band has been derived while the electron is interacting with a random, but inhomogeneous distribution of impurities, and is subject to general homogeneous and inhomogeneous electric fields. The quantum transport equation for the Wigner distribution function is derived from the Liouville equation; in this problem, the Bloch electrons in a single band are described by an effective Hamiltonian interacting with a random, but inhomogeneous distribution of elastic scatterers in the simultaneous presence of an inhomogeneous time-dependent potential and a homogeneous electric field of arbitrary magnitude and time dependence. The derivation of the transport equation makes use of a unitary transformation of the Liouville equation based on the interaction picture to one in which the scattering interaction appears quadradically. The basis states employed in evaluating the matrix elements of the transformed Liouville equation are the instantaneous eigenstates of the single band effective Hamiltonian which include the homogeneous electric field through the use of the vector potential gauge. The equation for the Wigner distribution function is derived from the transformed Liouville equation; the generalized drift and diffusion terms are obtained exactly for arbitrary band structure, and the collision integral is obtained to the second order in the strength of the scattering potential, the only approximation being the neglect of the inhomogeneous potential in the evaluation of the scattering matrix elements; taking the limit of slowly varying inhomogeneous electric field and slowly varying scatterer density distribution, a quantum generalization of the Boltzmann equation is obtained which includes *impurity-related* intracollisional field effects in the collision term and a drift term with a total force comprising the homogeneous and inhomogeneous fields.

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