Quantum transport for electron quasiparticles interacting with a disordered binary alloy: A Wigner approach

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Quantum transport is developed in the Wigner function representation for a Bloch electron quasiparticle interacting with a disordered binary alloy in the presence of a homogeneous electric field of arbitrary time dependence and amplitude. The electron quasiparticle is described by a single-band effective Hamiltonian, and the homogeneous electric field is treated in the vector potential gauge. The methodology for the quantum transport analysis proceeds by first transforming the Liouville equation to one in which the interaction Hamiltonian (the binary alloy Hamiltonian) appears quadratically. The basis states employed in evaluating the requisite matrix elements are the instantaneous eigenstates of the electron quasiparticle Hamiltonian in the presence of the electric field. The Wigner quantum transport equations are derived, and the binary alloy collision term is suitably ensemble averaged over the disordered binary alloy matrix elements. In addition, the general drift and diffusion terms are exactly obtained, resulting in the complete Wigner-Boltzmann equation for the binary alloy system. In approximating the collision term for the two separate cases of parabolic energy dispersion and the long-wavelength limit, it is found that the reduced Wigner-Boltzmann equation includes the manifestation of the intracollisional field effect and other quantum generalities. As a contrast to the actual random alloy treatment, attention is given to the canonical problem of quantum transport for a *virtual crystal* (VC). As an alternative to the random binary alloy scattering problem, the VC Hamiltonian adopted for this treatment is derived by *ensemble averaging* the random binary alloy Hamiltonian. The resulting Wigner transport equation for the VC case is descriptive of Bloch dynamics in a graded semiconductor alloy.

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I. INTRODUCTION

The challenge of describing electron dynamics in a semiconductor where the Bloch bands are influenced by compositional alloying, as well as other constitutive modifications, has long been a cornerstone issue for many applications in solid-state physics. In this regard, the development of user-friendly formulations for treating alloy scattering, and compositionally tailored Bloch bands has had a long and useful history [1,2]. Needless to say, in addressing problems involving alloying and a degree of compositional disorder, it is often a matter of computational practicality to transition from a microscopic description to a suitable average of the problem that smoothes out the fluctuations inherit in the compositional disorder. Such is the situation, for example, when replacing the microscopic alloy potential energy by the so-called *virtual crystal approximation* (VCA) [3]. When such an averaging of practicality is involved, it is always natural to question the impact of such a transition on the quantum transport dynamics and on the dynamical variables of interest. In this work, we address such a consideration.

For purposes of this analysis, we consider the simplest model disordered binary alloy system of composition A_xB_{1-x} [1,2]. For the binary alloy model, it is assumed that the two constituent atoms of the alloy are ideally arranged on a periodic lattice in a random binary distribution; lattice distortions, and long/short-range correlations between the constituent atoms are neglected. The potential energy for the binary alloy model is expressed as

$$U(\mathbf{r},\{\mathbf{r}_i\}) = \sum_{\mathbf{r}_a}^{N_A} U_A(\mathbf{r}-\mathbf{r}_a) + \sum_{\mathbf{r}_b}^{N_B} U_B(\mathbf{r}-\mathbf{r}_b); \qquad (1)$$

here, with $N_A + N_B = N$, the constitutive atoms are randomly distributed over N perfectly periodic lattice sites, namely, $\mathbf{r}_a$ and $\mathbf{r}_b$ (which are otherwise random variables referred to as $\{\mathbf{r}_i\}$). Thus, although A and B posses potential energy $U_A(\mathbf{r})$ and $U_B(\mathbf{r})$ with the same periodicity, they are randomly distributed over N sites in a random binary configuration.

In this work, we consider the quantum dynamics for an electron described by a single-band effective Hamiltonian in a homogeneous electric field of arbitrary time dependence, interacting with an inhomogeneous potential energy of the disordered binary alloy of Eq. (1). As such, the total Hamiltonian is given by

$$\hat{H} = \hat{\varepsilon}_n(\hat{\mathbf{p}} + \mathbf{p}_c) + U(\mathbf{r},\{\mathbf{r}_i\}) + V(\mathbf{r}). \qquad (2)$$

Here, $\hat{\varepsilon}_n(\hat{\mathbf{p}} + \mathbf{p}_c)$ is the single-band effective Hamiltonian of the Bloch band $\varepsilon_n(\mathbf{K})$, $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}$ is the electron momentum operator, $U(\mathbf{r},\{\mathbf{r}_i\})$ is the binary alloy potential energy defined in Eq. (1), and $V(\mathbf{r})$ is an arbitrary external potential energy.

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In Sec. II, we develop the elements of the Liouville equation and the Wigner distribution function (WDF) [4] necessary to derive the Wigner-Boltzmann transport equation for the Hamiltonian of Eq. (2). The basis functions to be used in establishing the required matrix elements for this analysis will be the instantaneous eigenstates of $\hat{\varepsilon}_n(\hat{\mathbf{p}}+\mathbf{p}_c)$ in Eq. (2). The Liouville equation is utilized by transforming to an equivalent form in which the binary alloy term in Eq. (2) is treated quadratically. In Sec. III, we make use of the transformed Liouville equation to derive the Wigner-Boltzmann transport equation for the Hamiltonian of Eq. (2). The realized equation is then *ensemble averaged* over the binary distribution of the random variables $\{\mathbf{r}_i\}$ relevant to $U(\mathbf{r},\{\mathbf{r}_i\})$ in Eq. (2) to find the *ensemble averaged* Wigner-Boltzmann transport equation. The generalized drift and diffusion terms are exactly obtained. Noting the complexity of the collision term, we examine this term for the two separate approximate conditions of parabolic dispersion and the long-wavelength carrier limit to observe noted quantum effects. In Sec. IV, we take the ensemble average of the Hamiltonian in Eq. (2). This results in a *virtual crystal* (VC)-type of Hamiltonian; the Wigner-Boltzmann equation is developed for this VC Hamiltonian. The resulting Wigner-Boltzmann transport equation for the VC is descriptive of the Bloch dynamics in a single-band graded semiconductor alloy. In Sec. V, we summarize our results, emphasizing the importance of the ensemble averaging over random variables in quantum transport problems. In addition, the dynamical scenarios that emerge from the two different *ensemble averaging* sequences are causally addressed; it is shown from the Liouville equation that the density matrix and the interaction Hamiltonian possess different statistical correlation relations for the two different sequences which, in turn, gives rise to the different dynamical equations of motion.

II. LIOUVILLE EQUATION AND THE WIGNER FUNCTION REPRESENTATION

A. Liouville equation

In considering the problem of interest, we note that the Hamiltonian of Eq. (2) is expressed as a separation of kinetic and potential energy terms. Further, when considering an additional imposition of a spatially homogeneous, but arbitrarily time-dependent electric field, we previously showed [5–7] that this can be treated in the vector potential gauge by adding a time-dependent momentum $\mathbf{p}_c(t)$ to the mechanical momentum, so that

$$\hat{H}_0 = \hat{H}_0[\hat{\mathbf{p}}+\mathbf{p}_c(t)], \tag{3a}$$

where

$$\mathbf{p}_c(t) = \hbar\mathbf{k}_c(t) = e\int_{t_0}^{t}\mathbf{E}(t')dt'. \tag{3b}$$

Therefore, as a starting point for the quantum analysis, we begin with the Liouville equation for our system as

$$i\hbar\frac{\partial\hat{\varrho}}{\partial t} = [\hat{H}(\mathbf{r},\hat{\mathbf{p}},t),\hat{\varrho}] \equiv [\hat{H}_0[\hat{\mathbf{p}}+\mathbf{p}_c(t)]+\hat{H}'(\mathbf{r},t),\hat{\varrho}]. \tag{4}$$

It follows from time evolution treatment in our previous work [5] that Eq. (4) can be transformed conveniently with a unitary transformation $\hat{U}(t,t_0)$, defined by

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}_0[\hat{\mathbf{p}}+\mathbf{p}_c(t)]\hat{U}(t,t_0), \tag{5}$$

with $\hat{U}^+\hat{U} = \hat{U}\hat{U}^+ = \hat{1}$ and $\hat{U}(t,t')\hat{U}(t',t_0) = \hat{U}(t,t_0)$, so that

$$i\hbar\frac{\partial\hat{\varrho}}{\partial t} = [\hat{H}_0,\hat{\varrho}] + [\hat{H}'(t),\hat{U}(t,t_0)\hat{\varrho}(t_0)\hat{U}(t_0,t)] - \frac{i}{\hbar}\left[\hat{H}'(t),\int_{t_0}^{t}dt'\hat{U}(t,t')[\hat{H}'(t'),\hat{\varrho}(t')]\hat{U}(t',t)\right]. \tag{6}$$

It is noted that in the transformation from Eq. (4) to Eq. (6), the Liouville equation has separated the interaction term into two components, the first is *linear* in the interaction Hamiltonian $\hat{H}'$ and is characterized by the density matrix *initial condition*; the second term is *quadratic* in the interaction Hamiltonian and contains explicit quantum correlations of $\hat{\varrho}$ with $\hat{H}'$, along with temporal memory effects. Thus, we use Eq. (6) as a preferred form of the Liouville equation to develop the Wigner-Boltzmann quantum transport equations for our interest.

B. Wigner distribution function

In defining the single-particle WDF for our problem, which is generally a function of canonical variables $f(\mathbf{r},\mathbf{p},t)$, we take the Fourier transform of the single-particle density matrix in an appropriate basis. For this purpose, we use the instantaneous eigenstates of $\hat{\varepsilon}_n[-i\nabla_{\mathbf{r}}+\mathbf{k}_c(t)]$. The instantaneous eigenstate equation is then in the wave-vector $\mathbf{K}$ representation

$$\hat{\varepsilon}_n[-i\nabla_{\mathbf{r}}+\mathbf{k}_c(t)]|\mathbf{K}\rangle = \varepsilon_n[\mathbf{K}+\mathbf{k}_c(t)]|\mathbf{K}\rangle, \tag{7a}$$

where

$$|\mathbf{K}\rangle = \Omega^{-1/2}e^{i\mathbf{K}\cdot\mathbf{r}}, \tag{7b}$$

Ω is the normalization volume, $\mathbf{k}(\mathbf{K},t) = \mathbf{K}+\mathbf{k}_c(t)$, and $\mathbf{k}_c(t)$ is noted in Eq. (3b).

In determining the WDF for this analysis, we use the $|\mathbf{K}\rangle$ states of Eq. (7b) as a basis to establish the off-diagonal matrix elements [6] of $\hat{\varrho}$ to obtain $f(\mathbf{r},\mathbf{p},t)\rightarrow F(\mathbf{r},\mathbf{K},t)$ with $\mathbf{p} = \hbar\mathbf{K}$. Then

$$F(\mathbf{r},\mathbf{K},t) \equiv \Omega^{-1}\sum_{\mathbf{u}}\varrho_{\mathbf{K}+\mathbf{u}/2,\mathbf{K}-\mathbf{u}/2}(t)e^{i\mathbf{u}\cdot\mathbf{r}}, \tag{8}$$

where $\varrho_{\mathbf{K}\mathbf{K}'} \equiv \langle\mathbf{K}|\hat{\varrho}|\mathbf{K}'\rangle$. It follows that $F(\mathbf{r},\mathbf{K},t)$ satisfies the sum rules

$$\sum_{\mathbf{K}}F(\mathbf{r},\mathbf{K},t) = \varrho(\mathbf{r},t), \tag{9a}$$

where $\varrho(\mathbf{r},t)$ is the electron density and

$$\int_{\Omega}d\mathbf{r}F(\mathbf{r},\mathbf{K},t) = \varrho_{\mathbf{K}\mathbf{K}}(t). \tag{9b}$$

Kinematically, for any operator $\hat{B}$, we have the expectation value

$$\langle B\rangle \equiv Tr\{\hat{\varrho}\hat{B}\} = \sum_{\mathbf{K}}\int_{\Omega}d\mathbf{r}F(\mathbf{r},\mathbf{K})B_W(\mathbf{r},\mathbf{K}), \tag{10a}$$

where $B_W(\mathbf{r},\mathbf{K})$ is the Wigner-Weyl form for $\hat{B}$, given by

$$B_W(\mathbf{r},\mathbf{K}) = \Omega^{-1}\sum_{\mathbf{u}} B_{\mathbf{K}+\mathbf{u}/2,\mathbf{K}-\mathbf{u}/2}e^{i\mathbf{u}\cdot\mathbf{r}}. \tag{10b}$$

It then follows that for a local coordinate-dependent operator $\hat{B}(\mathbf{r})$, the equation for $\langle B\rangle$ in Eq. (10a) is further reduced to

$$\langle B\rangle = \sum_{\mathbf{K}}\int_{\Omega} d\mathbf{r}F(\mathbf{r},\mathbf{K})B_W(\mathbf{r}). \tag{11}$$

Alternatively, if $\hat{B}$ is diagonal in the $\mathbf{K}$ basis, i.e., $B_{\mathbf{K}\mathbf{K}'} = B_{\mathbf{K}}\delta_{\mathbf{K}\mathbf{K}'}$, then Eq. (10a) reduces to

$$\langle B\rangle = \sum_{\mathbf{K}}\int_{\Omega} d\mathbf{r}F(\mathbf{r},\mathbf{K})B_{\mathbf{K}}. \tag{12}$$

In using the Hamiltonian of Eq. (2) in Eq. (6) with $\hat{H}_0 = \hat{\varepsilon}_n[-i\nabla_{\mathbf{r}} + \mathbf{k}_c(t)] + V(\mathbf{r})$ and $\hat{H}' = U(\mathbf{r},\{\mathbf{r}_i\})$, we can take the required matrix elements and express the time rate of change of the WDF as

$$\frac{\partial}{\partial t}F(\mathbf{r},\mathbf{K},t) = T_\varepsilon + T_V + C_1 + C_2. \tag{13}$$

Here, from Eq. (10a), we see that T_ε and T_V become [5]

$$\begin{aligned} T_\varepsilon &= -\frac{i}{\hbar\Omega}\sum_{\mathbf{u}}[\varepsilon_n(\mathbf{k}+\mathbf{u}/2) - \varepsilon_n(\mathbf{k}-\mathbf{u}/2)]\varrho_{\mathbf{K}+\mathbf{u}/2,\mathbf{K}-\mathbf{u}/2} \\ &= -\frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[\varepsilon_n(\mathbf{K}+\mathbf{k}_c)F(\mathbf{r},\mathbf{K}')]_{\mathbf{K}'=\mathbf{K}} \end{aligned} \tag{14}$$

and

$$\begin{aligned} T_V &= -\frac{i}{\hbar\Omega}\sum_{\mathbf{u}}[V,\hat{\varrho}]_{\mathbf{K}+\mathbf{u}/2,\mathbf{K}-\mathbf{u}/2}e^{i\mathbf{u}\cdot\mathbf{r}} \\ &= \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[V(\mathbf{r})F(\mathbf{r}',\mathbf{K})]_{\mathbf{r}'=\mathbf{r}}. \end{aligned} \tag{15}$$

The last two terms in Eq. (13), namely C_1 and C_2, are derived from the linear and quadratic terms in H' of Eq. (6). As such, taking the required matrix elements, we find that

$$\begin{aligned} C_1 = \frac{1}{i\hbar\Omega}\sum_{\mathbf{u}}\Big\langle \mathbf{K}+\frac{\mathbf{u}}{2}\Big| \\ \times[\hat{H}'(t),\hat{U}(t,t_0)\hat{\varrho}(t_0)\hat{U}(t_0,t)]\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle e^{i\mathbf{u}\cdot\mathbf{r}}, \end{aligned} \tag{16}$$

$$\begin{aligned} C_2 = -\frac{1}{\hbar^2\Omega}\sum_{\mathbf{u}}\Big\langle \mathbf{K}+\frac{\mathbf{u}}{2}\Big|\Big[\hat{H}'(t),\int_{t_0}^{t}dt'\hat{U}(t,t') \\ \times[\hat{H}'(t'),\hat{\varrho}(t')]\hat{U}(t',t)\Big]\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle e^{i\mathbf{u}\cdot\mathbf{r}}. \end{aligned} \tag{17}$$

In the expression for C_1 of Eq. (16), the $\hat{\varrho}(t_0)$ dependence gives rise to off-diagonal initial conditions which are generally zero, however, see Appendix A for further discussion of $C_1(\mathbf{r},\mathbf{K},t)$. For C_2, expanding the outside commutator reveals that C_2 can be written as the sum of two terms $C_2 = C_2^{(1)} + C_2^{(2)}$, each term belonging to one of the terms of the expanded commutator. It thus follows that

$$\begin{aligned} C_2^{(1)} = -\frac{1}{\hbar^2\Omega}\int_{t_0}^{t}dt'\sum_{\mathbf{u}}\Big\langle \mathbf{K}+\frac{\mathbf{u}}{2}\Big|\hat{H}'(t)\hat{U}(t,t') \\ \times[\hat{H}'(t'),\hat{\varrho}(t')]\hat{U}(t',t)\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle e^{i\mathbf{u}\cdot\mathbf{r}}, \end{aligned} \tag{18a}$$

$$\begin{aligned} C_2^{(2)} = \frac{1}{\hbar^2\Omega}\int_{t_0}^{t}dt'\sum_{\mathbf{u}}\Big\langle \mathbf{K}+\frac{\mathbf{u}}{2}\Big|\hat{U}(t,t')[\hat{H}'(t'),\hat{\varrho}(t')] \\ \times\hat{U}(t',t)\hat{H}'(t)\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle e^{i\mathbf{u}\cdot\mathbf{r}}. \end{aligned} \tag{18b}$$

With regard to the explicit form of $\hat{U}(t,t_0)$ from Eq. (5), we note that we divided the full Hamiltonian of Eq. (2) into two parts in Eq. (4), namely, $\hat{H}_0 = \hat{\varepsilon}_n[-i\nabla_{\mathbf{r}} + \mathbf{k}_c(t)] + V(\mathbf{r})$ and $\hat{H}' = U(\mathbf{r},\{\mathbf{r}_i\})$. Here, $\hat{\varepsilon}_n[-i\nabla_{\mathbf{r}} + \mathbf{k}_c(t)]$ is chosen as the source of the instantaneous eigenstates from Eqs. (7a) and (7b). Then, in using Eq. (5) along with $\hat{U}_0$ defined by $i\hbar\partial\hat{U}_0/\partial t = \hat{\varepsilon}_n[-i\nabla_{\mathbf{r}} + \mathbf{k}_c(t)]\hat{U}_0$, it follows that

$$i\hbar\frac{\partial}{\partial t}(\hat{U}_0^\dagger\hat{U}) = \hat{U}_0^\dagger V(t)\hat{U}.$$

Upon integration, we obtain

$$\hat{U}(t,t_0) = \hat{U}_0(t,t_0)\Big\{\hat{I} - \frac{i}{\hbar}\int_{t_0}^{t}dt'\hat{U}_0(t_0,t')V(t')\hat{U}(t',t_0)\Big\},$$

an exact result for the given $\hat{U}_0$ above and $\hat{U}(t,t_0)$ from Eq. (5). But, as a first approximation, letting $\hat{U}(t,t_0)\approx\hat{U}_0(t,t_0)$ under the integral, and then taking the matrix elements with respect to $|\mathbf{K}\rangle$ of Eq. (7b), we find that

$$\begin{aligned} U_{\mathbf{K}\mathbf{K}'}(t,t_0) \approx e^{-\frac{i}{\hbar}\int_{t_0}^{t}\varepsilon_n[\mathbf{k}(\tau)]d\tau}\Bigg[\delta_{\mathbf{K}\mathbf{K}'} - \frac{i}{\hbar}\int_{t_0}^{t}dt'V_{\mathbf{K}\mathbf{K}'}(t') \\ \times e^{\frac{i}{\hbar}\int_{t_0}^{t'}\{\varepsilon_n[\mathbf{k}(\tau)]-\varepsilon_n[\mathbf{k}'(\tau)]\}\,d\tau}\Bigg]. \end{aligned}$$

Here, we see that $U_{\mathbf{K}\mathbf{K}'}$ contains the leading instantaneous eigenstate term, but also, in the second term, a higher-order term in the inhomogeneous external potential $V(\mathbf{r})$. Since we only focus attention on $U(\mathbf{r},\{\mathbf{r}_i\})$ in this work, we elect to retain only the lowest-order term in $U_{\mathbf{K}\mathbf{K}'}$ so that

$$U_{\mathbf{K}\mathbf{K}'}(t,t_0) \approx e^{-\frac{i}{\hbar}\int_{t_0}^{t}\varepsilon_n[\mathbf{k}(\tau)]d\tau}\delta_{\mathbf{K}\mathbf{K}'},$$

with $\hat{U}(t,t_0)\approx\hat{U}_0(t,t_0)$. This approximation is adopted from now on.

In Eq. (18a), inserting in between $\hat{H}'$ and $\hat{U}(t,t')$ the complete set of states representing by the term $\sum_{\mathbf{K}'}|\mathbf{K}'+\mathbf{u}/2\rangle\langle\mathbf{K}'+\mathbf{u}/2|$, and noting that

$$\begin{aligned} \Big\langle \mathbf{K}+\frac{\mathbf{u}}{2}\Big|\hat{H}'\Big|\mathbf{K}'+\frac{\mathbf{u}}{2}\Big\rangle = H'_{\mathbf{K}\mathbf{K}'}, \\ \hat{U}(t',t)\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle = e^{-\frac{i}{\hbar}\int_{t}^{t'}\varepsilon_n(\mathbf{k}(\tau)-\mathbf{u}/2)d\tau}\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle, \\ \Big\langle \mathbf{K}'+\frac{\mathbf{u}}{2}\Big|\hat{U}(t,t') = e^{\frac{i}{\hbar}\int_{t}^{t'}\varepsilon_n[\mathbf{k}'(\tau)+\mathbf{u}/2]d\tau}\Big\langle \mathbf{K}'+\frac{\mathbf{u}}{2}\Big|, \end{aligned} \tag{19}$$

we then get

$$C_2^{(1)} = -\frac{1}{\hbar^2\Omega}\sum_{\mathbf{u},\mathbf{K}'} H'_{\mathbf{K}\mathbf{K}'}(t)\int_{t_0}^{t} dt' \left\langle \mathbf{K}'+\frac{\mathbf{u}}{2}\middle|[\hat{H}'(t'),\hat{\varrho}(t')]\middle|\mathbf{K}-\frac{\mathbf{u}}{2}\right\rangle e^{\frac{i}{\hbar}\int_t^{t'}[\varepsilon_n[\mathbf{k}'(\tau)+\mathbf{u}/2]-\varepsilon_n[\mathbf{k}(\tau)-\mathbf{u}/2]d\tau} e^{i\mathbf{u}\cdot\mathbf{r}}. \tag{20}$$

Finally, expanding the commutator and using the expression for $F(\mathbf{r},\mathbf{K},t)$ defined in Eq. (8), we get for $C_2^{(1)} = C_2^{(1)}(\mathbf{r},\mathbf{K},t)$ above

$$C_2^{(1)} = -\frac{1}{\hbar^2\Omega}\sum_{\mathbf{u},\mathbf{K}',\mathbf{K}''} H'_{\mathbf{K}\mathbf{K}'}(t)\int_{t_0}^{t} dt' \left\{ H'_{\mathbf{K}'\mathbf{K}''}(t')\int_\Omega d\mathbf{r}' F\left(\mathbf{r}',\frac{\mathbf{K}''+\mathbf{K}}{2},t'\right) e^{-i(\mathbf{K}''-\mathbf{K})\cdot\mathbf{r}'} e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')} - H'_{\mathbf{K}''\mathbf{K}}(t') \right.$$
$$\left. \times \int_\Omega d\mathbf{r}' F\left(\mathbf{r}',\frac{\mathbf{K}'+\mathbf{K}''}{2},t'\right) e^{-i(\mathbf{K}'-\mathbf{K}'')\cdot\mathbf{r}'} e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')} \right\} e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon_n[\mathbf{k}'(\tau)+\mathbf{u}/2]-\varepsilon_n[\mathbf{k}(\tau)-\mathbf{u}/2]\}d\tau}. \tag{21}$$

Similarly, we find that the other term $C_2^{(2)}$ satisfies the relation $C_2^{(2)} = C_2^{(1)*}$. Thus, the term $C_2(\mathbf{r},\mathbf{K},t)$ is given by

$$C_2(\mathbf{r},\mathbf{K},t) = C_2^{(1)} + C_2^{(1)*} = 2ReC_2^{(1)}(\mathbf{r},\mathbf{K},t). \tag{22}$$

III. ELECTRON QUASIPARTICLE SCATTERED BY A RANDOM BINARY ALLOY

The time evolution of the Wigner function is defined by Eq. (13), with C_1 and C_2 given by Eqs. (16) and (22), respectively. Since the Wigner function $F(\mathbf{r},\mathbf{K},t)$ of Eq. (13) is dependent upon the random variables inherent in the potential energy of the binary alloy of Eq. (1), that is, the set $\{\mathbf{r}_i\}$, it is incumbent upon us to take the ensemble average of the Wigner equation over the appropriate random variables. Since these variables are explicitly introduced in $U_{A,B}$ of Eq. (1), they are subsequently found in the matrix elements of C_2 and C_1 (see Appendix A). We now focus on the Hamiltonian $\hat{H}'$ of Eq. (2), that is, $U(\mathbf{r},\{\mathbf{r}_i\})$, so as to calculate the appropriate matrix elements relevant to the C_2 term. Considering from Eq. (1), we now refer to $U(\mathbf{r},\{\mathbf{r}_i\})$ as $\hat{H}'$ for purposes of the analysis so that

$$U(\mathbf{r},\{\mathbf{r}_i\},t) \equiv \hat{H}'(\mathbf{r},t) = \sum_{\mathbf{r}_a}^{N_A} U_A(\mathbf{r}-\mathbf{r}_a,t) + \sum_{\mathbf{r}_b}^{N_B} U_B(\mathbf{r}-\mathbf{r}_b,t); \tag{23}$$

note we introduced a "t'' dependence into $U(\mathbf{r},\{\mathbf{r}_i\},t)$ to allow for a time-dependent tracking in subsequent analysis. For $N_A + N_B = N$, we then form $H'_{\mathbf{K}\mathbf{K}'}(t)H'_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t')$ for use in Eq. (21). Using $\hat{H}'(t)$ of Eq. (23), we can write

$$H'_{\mathbf{K}\mathbf{K}'}(t)H'_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t') = [U_A(t)]_{\mathbf{K}\mathbf{K}'}[U_A(t')]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} \sum_{\mathbf{r}_a}^{N_A} e^{-i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}_a} \sum_{\mathbf{r}_{a'}}^{N_A} e^{i(\mathbf{K}-\mathbf{K}'-\mathbf{q})\cdot\mathbf{r}_{a'}}$$
$$+ [U_B(t)]_{\mathbf{K}\mathbf{K}'}[U_B(t')]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} \sum_{\mathbf{r}_b}^{N_B} e^{-i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}_b} \sum_{\mathbf{r}_{b'}}^{N_B} e^{i(\mathbf{K}-\mathbf{K}'-\mathbf{q})\cdot\mathbf{r}_{b'}}$$
$$+ [U_A(t)]_{\mathbf{K}\mathbf{K}'}[U_B(t')]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} \sum_{\mathbf{r}_a}^{N_A} e^{-i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}_a} \sum_{\mathbf{r}_b}^{N_B} e^{i(\mathbf{K}-\mathbf{K}'-\mathbf{q})\cdot\mathbf{r}_b}$$
$$+ [U_B(t)]_{\mathbf{K}\mathbf{K}'}[U_A(t')]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} \sum_{\mathbf{r}_b}^{N_B} e^{-i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}_b} \sum_{\mathbf{r}_a}^{N_A} e^{i(\mathbf{K}-\mathbf{K}'-\mathbf{q})\cdot\mathbf{r}_a}. \tag{24a}$$

Here,

$$[U_i(t)]_{\mathbf{K}\mathbf{K}'} = \int_\Omega U_i(\mathbf{r},t) e^{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}} d\mathbf{r}, \tag{24b}$$

with $i = (A,B)$, independent of $\mathbf{r}_a$ or $\mathbf{r}_b$, respectively.

We seek to evaluate the statistical ensemble average of Eq. (24a), namely, $\langle H'_{\mathbf{K}\mathbf{K}'}(t)H'_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t')\rangle$. This requires suitable configuration averaging over the random variables $\mathbf{r}_a$ and $\mathbf{r}_b$ in Eq. (24a), or the exponential sums over $\mathbf{r}_a$ and $\mathbf{r}_b$ therein. Such configuration averaging is given in Appendix B using the relevant assumption about a Gaussian distribution of the random variables. In this regard, in evaluating such a sum in Eq. (24a), we generally seek spatial averages of the form

$$\langle S_A\rangle = N_A \int d\mathbf{r}_a e^{i\boldsymbol{\alpha}_a\cdot\mathbf{r}_a}\rho(r_a), \tag{25a}$$

$$\langle S_B\rangle = N_B \int d\mathbf{r}_b e^{i\boldsymbol{\alpha}_b\cdot\mathbf{r}_b}\rho(r_b). \tag{25b}$$

It is noted that integrals of the type of Eqs. (25a) and (25b) can be evaluated exactly for the Gaussian distribution [8–10] function [Appendix B, Eq. (B2a)]; as such

$$I = \int d\mathbf{r} e^{\pm i\boldsymbol{\alpha}\cdot\mathbf{r}}\rho(r) = e^{-\alpha^2/4\beta}, \tag{26}$$

where $\boldsymbol{\alpha} = \boldsymbol{\alpha}_{a,b}$ and $\beta = \beta_{A,B}$, respectively and for the sums of Eq. (24a), $\boldsymbol{\alpha} = |\mathbf{K} - \mathbf{K}'|$ or $|\mathbf{K} - \mathbf{K}' - \mathbf{q}|$. Therefore, we can express the ensemble average of Eq. (24a) as

$$\langle H'_{\mathbf{K}\mathbf{K}'}(t)H'_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t')\rangle = N^2 n(\mathbf{K}-\mathbf{K}')n(\mathbf{K}-\mathbf{K}'-\mathbf{q})(C^2[U_A(t)]_{\mathbf{K}\mathbf{K}'}[U_A(t')]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} + (1-C)^2[U_B(t')]_{\mathbf{K}\mathbf{K}'}[U_B(t)]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} + C(1-C)\{[U_A(t')]_{\mathbf{K}\mathbf{K}'}[U_B(t)]_{\mathbf{K}',\mathbf{K}-\mathbf{q}} + [U_B(t')]_{\mathbf{K}\mathbf{K}'}[U_A(t)]_{\mathbf{K}',\mathbf{K}-\mathbf{q}}\}). \tag{27}$$

Here $C = N_A/N$, $1 - C = N_B/N$, $N_A + N_B = N$, and $n(\mathbf{Q}) = \exp(-|\mathbf{Q}|N\langle r^2\rangle/6)$. Also, of course, since $U(\mathbf{r}, \{\mathbf{r}_i\}, t)$ in Eqs. (23) and (24a) is actually a function of $\mathbf{r}$ alone, $U = U(\mathbf{r}, \{\mathbf{r}_i\})$, then Eq. (24a) is time independent, so that $t = t' = t_0$ for this case; but we inserted "t'' dependence for purposes of generality in utilizing C_2 in Eq. (22) and in tracking matrix elements analysis.

We note that Eq. (27) can be re-expressed in direct compact form with $t = t' = t_0$ as

$$\langle H'_{\mathbf{K}\mathbf{K}'}(t)H'_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t')\rangle = \Phi_{\mathbf{K}\mathbf{K}'}(t_0)\Phi_{\mathbf{K}',\mathbf{K}-\mathbf{q}}(t_0), \tag{28a}$$

where

$$\Phi_{\mathbf{K}\mathbf{K}'}(t_0) = Nn(\mathbf{K}-\mathbf{K}')\{C[U_A(t_0)]_{\mathbf{K}\mathbf{K}'} + (1-C)[U_B(t_0)]_{\mathbf{K}\mathbf{K}'}\}. \tag{28b}$$

Then, inserting the time-independent ensemble average of Eqs. (28a) and (28b) into the scattering term of Eq. (21), we obtain for Eq. (22)

$$C_2(\mathbf{r},\mathbf{K},t) = \frac{2}{\hbar^2\Omega}Re\sum_{\mathbf{u},\mathbf{K}',\mathbf{q}}\Phi_{\mathbf{K}\mathbf{K}'}\int_{t_0}^{t}dt'\Bigg\{\Phi_{\mathbf{K}'+\mathbf{q},\mathbf{K}}\int_\Omega d\mathbf{r}' F\left(\mathbf{r}',\mathbf{K}'+\frac{\mathbf{q}}{2},t'\right)e^{i\mathbf{q}\cdot\mathbf{r}'}e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')} - \Phi_{\mathbf{K}',\mathbf{K}-\mathbf{q}}\int_\Omega d\mathbf{r}' F\left(\mathbf{r}',\mathbf{K}-\frac{\mathbf{q}}{2},t'\right)e^{i\mathbf{q}\cdot\mathbf{r}'}e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')}\Bigg\}e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon[\mathbf{k}'(\tau)+\mathbf{u}/2]-\varepsilon[\mathbf{k}(\tau)-\mathbf{u}/2]\}d\tau}. \tag{29}$$

Here, $\Phi_{\mathbf{K}\mathbf{K}'}$ and $\Phi_{\mathbf{K}',\mathbf{K}-\mathbf{q}}$ are time independent as being inferred from Eqs. (28a) and (28b). Thus, from Eqs. (13) and (29), we can write the Wigner equation for the binary alloy Hamiltonian of Eq. (2) [taken as Eq. (13) with $C_1 = C_1(\mathbf{r},\mathbf{K},t)$] as

$$\frac{\partial}{\partial t}F(\mathbf{r},\mathbf{K},t) + \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[\varepsilon(\mathbf{K}+\mathbf{k}_c)F(\mathbf{r},\mathbf{K}')]_{\mathbf{K}'=\mathbf{K}} = C_2(\mathbf{r},\mathbf{K},t) + C_1(\mathbf{r},\mathbf{K},t), \tag{30}$$

where $C_2(\mathbf{r},\mathbf{K},t)$ is given in Eq. (29), and we omit the band index n for purposes of notational brevity. In transforming to gauge invariant variables [6], we transform the Wigner equation (30) from $(\mathbf{K},t)$ variables to $[\mathbf{k}(t),t]$ variables using the transformation equations

$$\mathbf{k}(t) = \mathbf{K} + \mathbf{k}_c(t) = \mathbf{K} + \frac{e}{\hbar}\int_{t_0}^{t}\mathbf{E}(t')dt', \tag{31a}$$

$$W[\mathbf{r},\mathbf{k}(t),t] = F(\mathbf{r},\mathbf{K},t). \tag{31b}$$

It then follows that

$$\frac{\partial}{\partial t}F(\mathbf{r},\mathbf{K},t) = \frac{\partial}{\partial t}W(\mathbf{r},\mathbf{k},t) + \hbar^{-1}e\mathbf{E}\cdot\nabla_{\mathbf{k}}W(\mathbf{r},\mathbf{k},t),$$
$$\nabla_{x_i}F(\mathbf{r},\mathbf{K},t) = \nabla_{x_i}W(\mathbf{r},\mathbf{k},t).$$

Thus, the Wigner equation (30) becomes

$$\frac{\partial}{\partial t}W(\mathbf{r},\mathbf{k},t) + \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{k}})[\varepsilon(\mathbf{k})W(\mathbf{r},\mathbf{k}',t)]_{\mathbf{k}'=\mathbf{k}} + \hbar^{-1}e\mathbf{E}\cdot\nabla_{\mathbf{k}}W(\mathbf{r},\mathbf{k},t) = C_2(\mathbf{r},\mathbf{k},t) + C_1(\mathbf{r},\mathbf{k},t). \tag{32}$$

Here, $C_2(\mathbf{r},\mathbf{k},t)$ transforms from Eq. (29) as

$$C_2(\mathbf{r},\mathbf{k},t) = \frac{2}{\hbar^2\Omega}\mathrm{Re}\sum_{\mathbf{u},\mathbf{k}',\mathbf{q}}\Phi_{\mathbf{k}\mathbf{k}'}\int_{t_0}^{t}dt'\Bigg\{\Phi_{\mathbf{k}'+\mathbf{q},\mathbf{k}}\int_\Omega d\mathbf{r}' W \times\left(\mathbf{r}',\mathbf{k}'+\frac{\mathbf{q}}{2},t'\right)e^{i\mathbf{q}\cdot\mathbf{r}'}e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')} - \Phi_{\mathbf{k}',\mathbf{k}-\mathbf{q}} \times\int_\Omega d\mathbf{r}' W\left(\mathbf{r}',\mathbf{k}-\frac{\mathbf{q}}{2},t'\right)e^{i\mathbf{q}\cdot\mathbf{r}'}e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')}\Bigg\} \times e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon[\mathbf{k}'(\tau)+\mathbf{u}/2]-\varepsilon[\mathbf{k}(\tau)-\mathbf{u}/2]\}d\tau}. \tag{33}$$

The collision term (33) in Eq. (32) adds substantial complication to the solution of the equation, requiring sums over $\mathbf{u}$, $\mathbf{q}$, and $\mathbf{k}'$ as well as integrals over $\mathbf{r}'$ and t'. However, in key approximate physical limits, significant insight and simplicity is revealed. Such approximations are now considered for both $\mathbf{q} \simeq 0$ [11] and the parabolic energy dispersion. In neglecting the dependence on $\mathbf{q}$ in both the matrix elements and W in Eq. (33) and summing the remaining terms over $\mathbf{q}$ and $\mathbf{u}$, we find

$$C_2(\mathbf{r},\mathbf{k},t) \approx \frac{2}{\hbar^2}\mathrm{Re}\sum_{\mathbf{k}'}|\Phi_{\mathbf{k}\mathbf{k}'}|^2\int_{t_0}^{t}dt'[W[\mathbf{r},\mathbf{k}'(t'),t'] - W[\mathbf{r},\mathbf{k}(t'),t']]e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau]\}d\tau}, \tag{34a}$$

where

$$|\Phi_{\mathbf{k}\mathbf{k}'}|^2 = |Nn(\mathbf{K}-\mathbf{K}')[C(U_A)_{\mathbf{K}\mathbf{K}'} + (1-C)(U_B)_{\mathbf{K}\mathbf{K}'}]|^2. \tag{34b}$$

We note that $C_2(\mathbf{r},\mathbf{k},t)$ in Eq. (34a) is the generalization of the Boltzmann scattering term, including the *intracollisional field effect*, and the average matrix elements are the matrix elements of the binary distribution of the constituent potential energies, U_A and U_B.

On the other hand, for the case of parabolic energy dispersion, we have

$$\varepsilon(\mathbf{k}'(\tau)+\mathbf{u}/2) - \varepsilon(\mathbf{k}(\tau)-\mathbf{u}/2) \approx \varepsilon[\mathbf{k}'(\tau)] - \varepsilon[\mathbf{k}(\tau)] + \tfrac{1}{2}[\nabla_{\mathbf{k}'}\varepsilon[\mathbf{k}'(\tau)] + \nabla_{\mathbf{k}}\varepsilon[\mathbf{k}(\tau)]]\cdot\mathbf{u}, \tag{35}$$

so that

$$\begin{aligned}\frac{1}{\hbar}\int_t^{t'} &[\varepsilon[\mathbf{k}'(\tau)+\mathbf{u}/2] - \varepsilon[\mathbf{k}(\tau)-\mathbf{u}/2]]d\tau \\ &\approx \frac{1}{\hbar}\int_t^{t'}[\varepsilon[\mathbf{k}'(\tau)] - \varepsilon[\mathbf{k}(\tau)]]d\tau \\ &\quad + \frac{1}{2}\int_t^{t'} d\tau[\mathbf{v}[\mathbf{k}'(\tau)] - \mathbf{v}[\mathbf{k}(\tau)]]\cdot\mathbf{u} \\ &\equiv \frac{1}{\hbar}\int_t^{t'}[\varepsilon[\mathbf{k}'(\tau)] - \varepsilon[\mathbf{k}(\tau)]]d\tau + \bar{\mathbf{r}}(\mathbf{k},\mathbf{k}';t,t')\cdot\mathbf{u};\end{aligned} \tag{36a}$$

here

$$\bar{\mathbf{r}}(\mathbf{k},\mathbf{k}';t,t') = \frac{1}{2}\int_t^{t'} d\tau[\mathbf{v}[\mathbf{k}'(\tau)] - \mathbf{v}[\mathbf{k}(\tau)]]. \tag{36b}$$

Therefore, $C_2(\mathbf{r},\mathbf{k},t)$ of Eq. (33) takes on a $\mathbf{u}$-term containing the sum

$$\Omega^{-1}\sum_{\mathbf{u}} e^{i\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}'-\bar{\mathbf{r}})} = \delta(\mathbf{r}-\mathbf{r}'-\bar{\mathbf{r}}),$$

so that the integral over $\mathbf{r}'$ can be evaluated in Eq. (33) to obtain

$$\begin{aligned}C_2(\mathbf{r},\mathbf{k},t) = \frac{2}{\hbar^2}\mathrm{Re}\sum_{\mathbf{k}',\mathbf{q}}\Phi_{\mathbf{k}\mathbf{k}'}\int_{t_0}^{t}dt' &\times\left\{\Phi_{\mathbf{k}'+\mathbf{q},\mathbf{k}}W\left(\mathbf{r}-\bar{\mathbf{r}},\mathbf{k}'+\frac{\mathbf{q}}{2},t'\right)\right. \\ &\left. - \Phi_{\mathbf{k}',\mathbf{k}-\mathbf{q}}W\left(\mathbf{r}-\bar{\mathbf{r}},\mathbf{k}-\frac{\mathbf{q}}{2},t'\right)\right\} \\ &\times e^{i\mathbf{q}\cdot(\mathbf{r}-\bar{\mathbf{r}})}e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau)]\}d\tau}.\end{aligned} \tag{37}$$

We note that Eq. (37) is a generalization of a result due to Price [12]. As noted by Price, we conclude that in the weak field limit, $\bar{\mathbf{r}}$ of Eq. (36b) is of the order of a typical de Broglie wavelength so that its appearance in Eq. (37) will be significant only if $W(\mathbf{r},\mathbf{k},t)$ changes appreciably over such a dimension.

As a final consideration, we note that in Eqs. (34a) and (37), the implicit manifestation of the intracollisional field effect appears in the term

$$\mathcal{I} = e^{\frac{i}{\hbar}\int_t^{t'}\{\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau)]d\tau}. \tag{38a}$$

The effect refers to the explicit inclusion of the acceleration of the electron by the external field during the collision process in accordance with Eq. (31) [13]. As an example, using the effective mass approximation for the energy dispersion $\varepsilon(\mathbf{K}) = \hbar^2K^2/2m^*$, along with Eq. (31), we find that

$$\mathcal{I} = e^{\frac{i}{\hbar}[\varepsilon(\mathbf{K}')-\varepsilon(\mathbf{K})](t'-t)+i\beta(t',t)}, \tag{38b}$$

where

$$\beta(t',t) = [\mathbf{v}(\mathbf{K}')-\mathbf{v}(\mathbf{K})]\cdot\int_t^{t'}\mathbf{k}_c(\tau)d\tau. \tag{38c}$$

Here, $\mathbf{v}(\mathbf{K}) = \hbar\mathbf{K}/m^*$ is the effective mass velocity and $\mathbf{k}_c(\tau)$ is given in Eq. (31) as $\mathbf{k}_c(\tau) = (e/\hbar)\int_0^{\tau}\mathbf{E}(t')dt'(t_0=0)$. In the constant electric field, $\mathbf{E}=\mathbf{E}_0$, so that $\mathbf{k}_c(\tau) = (e/\hbar)\mathbf{E}_0\tau$ and

$$\beta(t',t) = (e/2\hbar)\mathbf{E}_0\cdot[\mathbf{v}(\mathbf{K}')-\mathbf{v}(\mathbf{K})](t'^2-t^2). \tag{38d}$$

$\beta(t',t)$ is noted in Eq. (38d) as the *broadening parameter* [14], as it introduces collision broadening into the scattering and transition processes as the electric field increases, but it is simply the power absorbed from the electric field during the collision duration.

IV. ENSEMBLE AVERAGED HAMILTONIAN: VIRTUAL HAMILTONIAN

The Hamiltonian of Eq. (2) is an explicit function of random variables $\{\mathbf{r}_i\}$. In this regard, it is instructive to perform an ensemble average of the Hamiltonian over the random variables in much the same way we ensemble averaged the collision term C_2 in Sec. III. Since the random variables are contained in $\hat{H}'$, where

$$\hat{H}'(\mathbf{r},\{\mathbf{r}_i\}) = \sum_{\mathbf{r}_a}^{N_A}U_A(\mathbf{r}-\mathbf{r}_a) + \sum_{\mathbf{r}_b}^{N_B}U_B(\mathbf{r}-\mathbf{r}_b), \tag{39}$$

we form the ensemble average as

$$\langle\hat{H}'\rangle = \int d\mathbf{r}_1 d\mathbf{r}_2\ldots d\mathbf{r}_N\hat{H}'(\mathbf{r},\{\mathbf{r}_i\})\rho(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N). \tag{40}$$

Here, the probability density is $\rho(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) = \rho(\mathbf{r}_1)\rho(\mathbf{r}_2)\ldots\rho(\mathbf{r}_N)$, while $\rho(\mathbf{r}_i)$ is defined in Eq. (B2a) of Appendix A, with

$$\int d\mathbf{r}_i\rho(\mathbf{r}_i) = 1.$$

Then, it follows that

$$\begin{aligned}\langle\hat{H}'\rangle &= N_A\int U_A(\mathbf{r}-\mathbf{r}_a)\rho(\mathbf{r}_a)d\mathbf{r}_a \\ &\quad + N_B\int U_B(\mathbf{r}-\mathbf{r}_b)\rho(\mathbf{r}_b)d\mathbf{r}_b \\ &= N[C\bar{U}_A(\mathbf{r}) + (1-C)\bar{U}_B(\mathbf{r}],\end{aligned} \tag{41a}$$

where

$$\bar{U}_A(\mathbf{r}) = \int U_A(\mathbf{r}-\mathbf{r}_a)\rho(\mathbf{r}_a)d\mathbf{r}_a, \tag{41b}$$

$$\bar{U}_B(\mathbf{r}) = \int U_B(\mathbf{r}-\mathbf{r}_b)\rho(\mathbf{r}_b)d\mathbf{r}_b. \tag{41c}$$

$U_{A/B}(\mathbf{r})$ of Eqs. (41b) and (41c) can be further expanded by noting that both potential energies are periodic with the same periodicity. Thus, they can be expanded in terms of the same type of reciprocal-lattice Fourier series as

$$U_{A/B}(\mathbf{r}) = \sum_{\mathbf{G}} A_{\mathbf{G}}/B_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}, \tag{42a}$$

where

$$A_{\mathbf{G}}/B_{\mathbf{G}} = \Omega^{-1}\int d\mathbf{r} U_{A/B}(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}}, \tag{42b}$$

Then, using Eq. (42a) in Eq. (41b), it follows, after integration while using $\varrho(r_a)$ of Eq. (B2a) that

$$\bar{U}_A(\mathbf{r}) = \int_{\Omega} d\mathbf{r}' U_A(\mathbf{r}') T_A(\mathbf{r}-\mathbf{r}'); \tag{43a}$$

here

$$T_A(\mathbf{r}-\mathbf{r}') = \Omega^{-1}\sum_{\mathbf{G}} e^{i\mathbf{G}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\mathbf{G}^2/4\beta_A}, \tag{43b}$$

with $(4\beta_A)^{-1} = N_A\langle r^2\rangle/6$. $T_A(\mathbf{r}-\mathbf{r}')$ of Eq. (43b) is a Gaussian reciprocal lattice sum and can be expanded as a lattice sum through the method of Poisson sum rule to yield

$$\Omega^{-1}\sum_{\mathbf{G}} e^{i\mathbf{G}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\mathbf{G}^2/4\beta_A} = \left(\frac{\beta_A}{\pi}\right)^{3/2}\sum_{\mathbf{l}} e^{-|\mathbf{l}-(\mathbf{r}-\mathbf{r}')|^2\beta_A}, \tag{44}$$

where $\mathbf{l}$ is the lattice vector space. It is noted that the right-hand side of Eq. (44) is recognized as a *translated-lattice "theta function"* [15].

Using the result of Eq. (44) in Eq. (43b), we find that

$$T_{A/B}(\mathbf{r}-\mathbf{r}') = \left(\frac{\beta_{A/B}}{\pi}\right)^{3/2}\sum_{\mathbf{l}} e^{-|\mathbf{l}-(\mathbf{r}-\mathbf{r}')|^2\beta_{A/B}}. \tag{45a}$$

Here, $T_{A/B}(\mathbf{r})$ is periodic with the lattice and

$$(4\beta_{A/B})^{-1} = N_{A/B}\langle r^2\rangle/6; \tag{45b}$$

then Eqs. (41b) and (41c) can be expressed as

$$\bar{U}_{A/B}(\mathbf{r}) = \int_{\Omega} d\mathbf{r}' U_{A/B}(\mathbf{r}') T_{A/B}(\mathbf{r}-\mathbf{r}'), \tag{46}$$

with $T_{A/B}(\mathbf{r}-\mathbf{r}')$ given by Eqs. (45a) and (45b).

Comparatively noting, while the collision matrix elements yielded an ensemble average of matrix elements, $|\Phi_{\mathbf{k}\mathbf{k}'}|$, in Eq. (34b), the ensemble average of $\hat{H}'$ gives a spatial average dependent upon the $U_{A/B}(\mathbf{r})$ of Eq. (46) expressed in Eq. (41a). We then observe that the full Hamiltonian of Eq. (2), when ensemble averaged, becomes

$$\langle\hat{H}\rangle = \hat{\varepsilon}_n(\mathbf{p}+\mathbf{p}_c) + N[C\bar{U}_A(\mathbf{r}) + (1-C)\bar{U}_B(\mathbf{r})] + V(\mathbf{r}), \tag{47}$$

which is akin to a VC-like Hamiltonian.

In developing the Wigner-Boltzmann equation for $\langle\hat{H}\rangle$, it is convenient to note that $\langle\hat{H}\rangle$ can be expressed equivalently as

$$\begin{aligned}\langle\hat{H}\rangle &= C[\hat{\varepsilon}_n(\mathbf{p}+\mathbf{p}_c) + N\bar{U}_A(\mathbf{r})] \\ &\quad + (1-C)[\hat{\varepsilon}_n(\mathbf{p}+\mathbf{p}_c) + N\bar{U}_B(\mathbf{r})] + V(\mathbf{r}) \\ &\equiv C\hat{H}_A + (1-C)\hat{H}_B + V(\mathbf{r}),\end{aligned} \tag{48a}$$

where

$$\hat{H}_A(\mathbf{r},\mathbf{p},t) = \hat{\varepsilon}_n[\mathbf{p}+\mathbf{p}_c(t)] + N\bar{U}_A(\mathbf{r}), \tag{48b}$$

$$\hat{H}_B(\mathbf{r},\mathbf{p},t) = \hat{\varepsilon}_n[\mathbf{p}+\mathbf{p}_c(t)] + N\bar{U}_B(\mathbf{r}). \tag{48c}$$

The *ensemble averaged* Hamiltonian of Eq. (48a) gives rise to a dynamical picture envisioned in the early development of semiconductors with nonuniform bands [16,17]. As such, we form the Wigner equation for $\langle\hat{H}\rangle$ of Eq. (48a). Noting from Eqs. (14) and (15), we see that, in the phase-space variables $(\mathbf{r},\mathbf{K},t)$, $F(\mathbf{r},\mathbf{K},t)$ satisfies

$$\frac{\partial F}{\partial t} = T_\varepsilon + T_U + T_V, \tag{49a}$$

where

$$T_\varepsilon = -\frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[\varepsilon(\mathbf{K}+\mathbf{k}_c)F(\mathbf{r},\mathbf{K}',t)]_{\mathbf{K}'=\mathbf{K}}, \tag{49b}$$

$$\begin{aligned}T_U = \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[N[C\bar{U}_A(\mathbf{r}) \\ + (1-C)\bar{U}_B(\mathbf{r})]F(\mathbf{r}',\mathbf{K},t)]_{\mathbf{r}'=\mathbf{r}},\end{aligned} \tag{49c}$$

and

$$T_V = \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{K}})[V(\mathbf{r})F(\mathbf{r}',\mathbf{K},t)]_{\mathbf{r}'=\mathbf{r}}. \tag{49d}$$

The results obtained in Eqs. (49a) to (49d) are expressed in terms of variables $(\mathbf{r},\mathbf{K},t)$. We now transform the results to a more conventional, gauge-invariant representation [6], with the new set of variables $[\mathbf{r},\mathbf{k}(t),t]$ using the transformation equations (31a) and (31b). Then it follows that

$$\frac{\partial}{\partial t}F(\mathbf{r},\mathbf{K},t) = \frac{\partial}{\partial t}W(\mathbf{r},\mathbf{k},t) + \frac{1}{\hbar}e\mathbf{E}(t)\cdot\nabla_{\mathbf{k}}W(\mathbf{r},\mathbf{k},t). \tag{50}$$

Thus, the Wigner-Boltzmann transport equation in Eq. (49a) becomes

$$\frac{\partial}{\partial t}W(\mathbf{r},\mathbf{k},t) + \frac{1}{\hbar}e\mathbf{E}(t)\cdot\nabla_{\mathbf{k}}W(\mathbf{r},\mathbf{k},t) - T'_\varepsilon - T'_U - T'_V = 0, \tag{51a}$$

where T'_ε, T'_U, and T'_V are the transformed functions given by

$$T'_\varepsilon = -\frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{k}})[\varepsilon(\mathbf{k})W(\mathbf{r},\mathbf{k}',t)]_{\mathbf{k}'=\mathbf{k}}, \tag{51b}$$

$$\begin{aligned}T'_U = \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{k}})[N[C\bar{U}_A(\mathbf{r}) \\ + (1-C)\bar{U}_B(\mathbf{r})]W(\mathbf{r}',\mathbf{k},t)]_{\mathbf{r}'=\mathbf{r}},\end{aligned} \tag{51c}$$

and

$$T'_V = \frac{1}{\hbar}\sin(\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{k}})[V(\mathbf{r})W(\mathbf{r}',\mathbf{k},t)]_{\mathbf{r}'=\mathbf{r}}. \tag{51d}$$

In the limit where the potential terms are slowly varying in space, we can approximate T'_ε, T'_U, and T'_V by retaining only the first term in the expansion of $\sin(\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{k}})$; then Eq. (51a) becomes

$$\frac{\partial}{\partial t} W(\mathbf{r}, \mathbf{k}, t) + \frac{1}{\hbar} \mathcal{F}(\mathbf{r}, t) \cdot \nabla_{\mathbf{k}} W(\mathbf{r}, \mathbf{k}, t) + \mathbf{v} \cdot \nabla_{\mathbf{r}} W(\mathbf{r}, \mathbf{k}, t) = 0, \tag{52a}$$

where

$$\mathcal{F}(\mathbf{r}, t) = e\mathbf{E}(t) - \nabla_{\mathbf{r}}[N[C\bar{U}_A(\mathbf{r}) + (1 - C)\bar{U}_B(\mathbf{r})]] - \nabla_{\mathbf{r}} V(\mathbf{r}) \tag{52b}$$

is the generalized force on the electron in the VC-like approximation and $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$ is the velocity. The generalized force affects the electron motion due to the applied force of the external electric field $e\mathbf{E}(t)$, but also has components which respond to both the gradient of the VC-potential energy and the arbitrary external potential energy $V(\mathbf{r})$. Particularly striking is the role of the gradient of the VC-potential energy since this component is exactly the type of internal force that affects the stimulated electron diffusion in nonuniform bands [16,17].

In the spirit of Wannier [18,19] and Slater [20], it is noted that if the Hamiltonian of Eqs. (48a) to (48c) is treated as a single-band Hamiltonian for the dynamics, then it follows that the wave-packet solution of the wave equation for the problem has the same trajectory as an electron motion derived from the analogous classical Hamiltons' equations. Therefore, we find that

$$\mathbf{v} = \nabla_{\mathbf{p}} \langle \hat{H}(\mathbf{r}, \mathbf{p}) \rangle = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k}) \tag{53}$$

and

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{r}} \langle \hat{H}(\mathbf{r}, \mathbf{p}) \rangle, \tag{54a}$$

which gives, using $\mathbf{p} = \hbar[\mathbf{k}(\mathbf{r}, t) - \mathbf{k}_c(t)]$ where $\hbar\mathbf{k}(\mathbf{r}, t)$ is the kinetic momentum and $\mathbf{k}_c(t)$ is given in Eq. (31),

$$\hbar\dot{\mathbf{k}}(\mathbf{r}, t) = e\mathbf{E}(t) - \nabla_{\mathbf{r}} \langle \hat{H}(\mathbf{r}, \mathbf{p}) \rangle = e\mathbf{E}(t) - \nabla_{\mathbf{r}}[N[C\bar{U}_A(\mathbf{r}) + (1 - C)\bar{U}_B(\mathbf{r})]] - \nabla_{\mathbf{r}} V(\mathbf{r}), \tag{54b}$$

the total $\mathbf{k}$-space force. Thus, the associated wave packet moves in $\mathbf{k}$-space according to Newton's second law [20]. These terms are borne out in the velocity and force terms of the collisionless Wigner-Boltzmann equation of Eq. (52a).

V. SUMMARY AND DISCUSSION

The quantum transport equations were developed in the Wigner function representation for a Bloch electron quasiparticle under the influence of a random binary alloy. The Bloch electron was subject to a homogeneous electric field of arbitrary strength and time dependence using the vector potential gauge. The electron quasiparticle was described by a single-band effective Hamiltonian which interacts with a binary alloy system.

The framework for developing the Wigner transport equations for the Hamiltonian of interest, including the appropriate basis states, was established. Treating the binary alloy Hamiltonian as a scattering component, the Wigner transport equation was established and ensemble averaged using an appropriate Gaussian distribution function. The formulation resulted in the exact drift and diffusion components, and scattering matrix elements which reflected the binary distribution of the constitutive binary atom matrix elements. Treating the scattering term in both the parabolic energy dispersion and long wavelength limits shows the explicit manifestation of the intracollisional field effect.

Lastly, we examine the Wigner transport dynamics for the ensemble averaged Hamiltonian. In this scenario, the binary potential energy term takes the form of a *virtual crystal*. The resulting Wigner transport equation is descriptive of Bloch electron dynamics in a graded single-band alloy.

It is striking to note that, in treating the binary alloy component of the Hamiltonian as a perturbative term, and then ensemble averaging the transport equation over the random alloy variables, we exposed the scattering picture of the transport; whereas, in ensemble averaging the Hamiltonian over the random alloy variables from the on-set, and then developing the requisite transport equation, we find that the binary alloy component has a band *renormalizing* influence on the behavior of the electron dynamics.

This difference in *ensemble average* sequencing is best appreciated by considering its effect on $\hat{\varrho}(t)$ of Eq. (4) or Eq. (6). When Eq. (4) is ensemble averaged over alloy random variables, we find that

$$i\hbar \frac{\partial \langle \hat{\varrho} \rangle}{\partial t} = [\hat{H}_0, \langle \hat{\varrho} \rangle] + \langle [\hat{H}', \hat{\varrho}] \rangle; \tag{55a}$$

here $\langle \ldots \rangle$ signifies the ensemble average. When Eq. (4) is ensemble averaged after $\hat{H}$, we then find that

$$i\hbar \frac{\partial \langle \hat{\varrho} \rangle}{\partial t} = [\hat{H}_0, \langle \hat{\varrho} \rangle] + [\langle \hat{H}' \rangle, \langle \hat{\varrho} \rangle]. \tag{55b}$$

One sees that in Eq. (55a), the averaging methods contains $\langle [\hat{H}', \hat{\varrho}] \rangle$, the fully correlated statistical relationship between $\hat{\varrho}$ and $\hat{H}'$; whereas, in Eq. (55b), the averaging procedure gives rise to $[\langle \hat{H}' \rangle, \langle \hat{\varrho} \rangle]$, a statistical independence between $\hat{\varrho}$ and $\hat{H}'$. Thus, the specific nature of the ensemble averaging affects the correlative relationship between $\hat{\varrho}$ and $\hat{H}'$, which, in turn, reflects the nature of the transport dynamical equation. In this effort, the ensemble average sequencing has resulted in a Wigner-Boltzmann quantum scattering picture, on the one hand, and a collisionless Wigner-Boltzmann semiclassical scenario, on the other.

APPENDIX A: DISCUSSION OF $C_1(\mathbf{r}, \mathbf{K}, t)$

In this discussion, we expand on the detailed evolution of the $C_1(\mathbf{r}, \mathbf{K}, t)$ term of Eq. (16). In opening the commutator and inserting a complete set of states through the use of

Eq. (19), we find that Eq. (16) takes the form

$$C_1(\mathbf{r},\mathbf{K},t)=\frac{1}{i\hbar\Omega}\sum_{\mathbf{K}',\mathbf{u}}[H'_{\mathbf{K}\mathbf{K}'}(t)\varrho_{\mathbf{K}'+\mathbf{u}/2,\mathbf{K}-\mathbf{u}/2}(t_0)e^{\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}'+\mathbf{u}/2)-\varepsilon(\mathbf{k}-\mathbf{u}/2)]d\tau}$$
$$-\varrho_{\mathbf{K}+\mathbf{u}/2,\mathbf{K}'-\mathbf{u}/2}(t_0)H'_{\mathbf{K}'\mathbf{K}}(t)e^{\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}+\mathbf{u}/2)-\varepsilon(\mathbf{k}'-\mathbf{u}/2)]d\tau}]e^{i\mathbf{u}\cdot\mathbf{r}}. \tag{A1}$$

Further, inverting Eq. (8), we get

$$\varrho_{\mathbf{K}_1\mathbf{K}_2}(t)=\int_\Omega d\mathbf{r}F(\mathbf{r},(\mathbf{K}_1+\mathbf{K}_2)/2,t)e^{-i(\mathbf{K}_1-\mathbf{K}_2)\cdot\mathbf{r}}. \tag{A2}$$

Inserting $\varrho_{\mathbf{K}_1\mathbf{K}_2}(t)$ of Eq. (A2) into Eq. (A1) with the appropriate $\mathbf{K}_1$ and $\mathbf{K}_2$, then Eq. (A1) becomes

$$C_1(\mathbf{r},\mathbf{K},t)=\frac{1}{i\hbar\Omega}\sum_{\mathbf{K}',\mathbf{u}}\int_\Omega d\mathbf{r}'F(\mathbf{r}',(\mathbf{K}+\mathbf{K}')/2,t_0)[H'_{\mathbf{K}\mathbf{K}'}(t)e^{i[(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}'+\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')]}e^{\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}'+\mathbf{u}/2)-\varepsilon(\mathbf{k}-\mathbf{u}/2)]d\tau}$$
$$-H'^{*}_{\mathbf{K}\mathbf{K}'}(t)e^{-i[(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}'-\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')]}e^{-\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}'-\mathbf{u}/2)-\varepsilon(\mathbf{k}+\mathbf{u}/2)]d\tau}]. \tag{A3}$$

We note that C_1 of Eq. (A3) is memory term dependent upon the Wigner distribution function at initial time t_0. Thus, when $C_1(\mathbf{r},\mathbf{K},t)$ is ensemble averaged over the scatterers in the Wigner-Boltzmann equation, the key determinant for the nonvanishing value of C_1 will be the average over $(\hat{H}'F)$ in Eq. (A3). In this regard, we point out that, in the scenario where the initial Wigner distribution function and $\hat{H}'(t)$ are uncorrelated, for example, should the electrons under consideration be injected initially into the dynamical process, then the ensemble average over C_1 would depend on $\hat{H}'$ alone. In this case, for discrete impurities [5], this ensemble average leads to $\langle H_{\mathbf{K}\mathbf{K}'}\rangle = N\Phi_{\mathbf{K}\mathbf{K}'}\delta_{\mathbf{K}\mathbf{K}'}$, diagonal matrix elements only, which can be absorbed into the energy function $\varepsilon(\mathbf{K})$; thus C_1 would vanish for the impurity scatterers case. Also, if as noted by Levinson [21] for the case of phonon scattering, a distribution at $t_0\to-\infty$ was arranged, which was completely uncorrelated with the position of the scatterers; then, for this situation, the ensemble average of our $C_1(\mathbf{r},\mathbf{K},t)$ would again be zero.

The examples above show that in many cases of interest it is practical, when applying the ensemble average methodology, to set $C_1(\mathbf{r},\mathbf{K},t)=0$. Nevertheless, we point out that for the binary alloy problem under consideration, we established from Eqs. (28a) and (28b) that $\langle\hat{H}'_{\mathbf{K}\mathbf{K}'}\rangle=\Phi_{\mathbf{K}\mathbf{K}'}=Nn(\mathbf{K}-\mathbf{K}')[C(U_A)_{\mathbf{K}\mathbf{K}'}+(1-C)(U_B)_{\mathbf{K}\mathbf{K}'}]$. Thus, even when assuming an uncorrelated Wigner function initially, the value for $\langle\hat{H}'_{\mathbf{K}\mathbf{K}'}\rangle=\Phi_{\mathbf{K}\mathbf{K}'}$ allows for the nonvanishing result for the ensemble average of $C_1(\mathbf{r},\mathbf{K},t)$.

Explicitly using $\langle\hat{H}'_{\mathbf{K}\mathbf{K}'}\rangle=\Phi_{\mathbf{K}\mathbf{K}'}$ in Eq. (A3), we can express the ensemble averaged $C_1(\mathbf{r},\mathbf{K},t)$ as

$$\langle C_1\rangle=\frac{1}{i\hbar\Omega}\sum_{\mathbf{K}',\mathbf{u}}[\Phi_{\mathbf{K}\mathbf{K}'}\int_\Omega d\mathbf{r}'F(\mathbf{r}',(\mathbf{K}+\mathbf{K}')/2,t_0)e^{i[(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}'+\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')]}e^{\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}'+\mathbf{u}/2)-\varepsilon(\mathbf{k}-\mathbf{u}/2)]d\tau}$$
$$-\Phi^{*}_{\mathbf{K}\mathbf{K}'}\int_\Omega d\mathbf{r}'F(\mathbf{r}',(\mathbf{K}+\mathbf{K}')/2,t_0)e^{-i[(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}'-\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}')]}e^{-\frac{i}{\hbar}\int_t^{t_0}[\varepsilon(\mathbf{k}'-\mathbf{u}/2)-\varepsilon(\mathbf{k}+\mathbf{u}/2)]d\tau}]. \tag{A4}$$

Although $\langle C_1\rangle$ in Eq. (A4) is generally nonvanishing, it is formidable to evaluate. Results can be simplified by considering the limit of parabolic energy dispersion as was treated in Eqs. (35) to (36b). Then we find that

$$\frac{1}{\hbar}\int_t^{t_0}[\varepsilon[\mathbf{k}'(\tau)\pm\mathbf{u}/2]-\varepsilon[\mathbf{k}(\tau)\mp\mathbf{u}/2]]d\tau\approx\frac{1}{\hbar}\int_t^{t_0}[\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau)]]d\tau\pm\bar{\mathbf{r}}(\mathbf{k},\mathbf{k}';t,t_0)\cdot\mathbf{u}, \tag{A5}$$

where $\bar{\mathbf{r}}$ is given in Eq. (36b). Using Eq. (A5) in Eq. (A4) and performing the sum over $\mathbf{u}$ and $\int_\Omega d\mathbf{r}'$, Eq. (A4) results in

$$\langle C_1\rangle=\frac{1}{i\hbar}\sum_{\mathbf{K}'}F[\mathbf{r}+\bar{\mathbf{r}},(\mathbf{K}+\mathbf{K}')/2,t_0]\{\Phi_{\mathbf{K}\mathbf{K}'}e^{i(\mathbf{K}-\mathbf{K}')\cdot(\mathbf{r}+\bar{\mathbf{r}})}e^{-\frac{i}{\hbar}\int_{t_0}^{t}\{\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau)]\}d\tau}-\Phi^{*}_{\mathbf{K}\mathbf{K}'}e^{-i(\mathbf{K}-\mathbf{K}')\cdot(\mathbf{r}+\bar{\mathbf{r}})}e^{\frac{i}{\hbar}\int_{t_0}^{t}\{\varepsilon[\mathbf{k}'(\tau)]-\varepsilon[\mathbf{k}(\tau)]\}d\tau}\}. \tag{A6}$$

Thus, for the binary alloy, we obtain an ensemble averaged $C_1(\mathbf{r},\mathbf{K},t)$ that depends explicitly on $\Phi_{\mathbf{K}\mathbf{K}'}$ and the initial value of the Wigner distribution function. Finally, since $F[\mathbf{r}+\bar{\mathbf{r}},(\mathbf{K}+\mathbf{K}')/2,t_0]$ is real due to the Hermiticity of $\hat{\varrho}$ [see Eq. (8)], Eq. (A6) can be expressed in a final compact form as

$$\langle C_1(\mathbf{r},\mathbf{K},t)\rangle=\frac{2}{\hbar}\sum_{\mathbf{K}'}F[\mathbf{r}+\bar{\mathbf{r}},(\mathbf{K}+\mathbf{K}')/2,t_0]\mathrm{Im}\{\Phi_{\mathbf{K}\mathbf{K}'}e^{i(\mathbf{K}-\mathbf{K}')\cdot(\mathbf{r}+\bar{\mathbf{r}})}e^{\frac{i}{\hbar}\int_{t_0}^{t}\{\varepsilon[\mathbf{k}(\tau)]-\varepsilon[\mathbf{k}'(\tau)]\}d\tau}\}. \tag{A7}$$

Equation (A7) can easily be expressed in terms of gauge invariant variable $W(\mathbf{r},\mathbf{k},t)$ through the use of Eqs. (31a) and (31b).

APPENDIX B: STATISTICAL ENSEMBLE AVERAGE

We consider as an example in an ensemble average over the random variable in Eq. (24a) the sum

$$S_A = \sum_{\mathbf{r}_a}^{N_A} e^{i\boldsymbol{\alpha}\cdot\mathbf{r}_a}. \tag{B1a}$$

In an ensemble average over $\mathbf{r}_a$, we let the ensemble average be represented as

$$\begin{aligned}\langle S_A\rangle &= \left\langle \sum_{\mathbf{r}_a}^{N_A} e^{i\boldsymbol{\alpha}\cdot\mathbf{r}_a}\right\rangle \\ &= \int d\mathbf{r}_{a_1} d\mathbf{r}_{a_2}\ldots d\mathbf{r}_{a_{N_A}}\rho\left(\mathbf{r}_{a_1},\mathbf{r}_{a_2},\ldots,\mathbf{r}_{a_{N_A}}\right) \\ &\quad\times\left[e^{i\boldsymbol{\alpha}_1\cdot\mathbf{r}_{a_1}}+e^{i\boldsymbol{\alpha}_2\cdot\mathbf{r}_{a_2}}+\ldots+e^{i\boldsymbol{\alpha}_{N_A}\cdot\mathbf{r}_{a_{N_A}}}\right]. \end{aligned}\tag{B1b}$$

Here, for a binomial distribution in the large N limit, $\rho(\mathbf{r}_{a_1},\mathbf{r}_{a_2},\ldots,\mathbf{r}_{a_N})$ is given by a Gaussian distribution, which, furthermore, can be expressed as a simple product of separate Gaussian distribution functions, that is, $\rho(\mathbf{r}_{a_1},\mathbf{r}_{a_2},\ldots,\mathbf{r}_{a_N}) = \rho(\mathbf{r}_{a_1})\rho(\mathbf{r}_{a_2})\ldots\rho(\mathbf{r}_{a_N})$. Thus, for a series of random variables $\mathbf{r}_{a_i}$, the integral of Eq. (B1b) can be expressed as N_A identical integrals

$$\langle S_A\rangle = N_A\int d\mathbf{r}_a e^{i\boldsymbol{\alpha}_a\cdot\mathbf{r}_a}\rho(r_a),$$

where $\boldsymbol{\alpha}_a$ is a given momentum transfer vector and $\rho(r_a)$ is a normalized, radially dependent Gaussian distribution function given by

$$\rho(r_a) = \left(\frac{\beta_A}{\pi}\right)^{3/2} e^{-\beta_A r_a^2}; \tag{B2a}$$

here

$$\beta_A = \frac{3}{2\langle r^2\rangle N_A}, \tag{B2b}$$

where $\langle r^2\rangle = N_A^{-1}\sum_{i=1}^{N_A} r_i^2$, the mean-square displacement resulting from the sum of displacements $\mathbf{r}_i$ in a random walk, with each displacement allowing for a random direction. The probability distribution function of Eq. (B2a) is a natural consequence of the application of stochastic methods to the problem of binomical distributions and random walks, and is thoroughly discussed in the seminal paper of Chandrasekhar [8] and others [9]. As such, in the large $N_{A,B}$ limit, Eq. (B2a) reflects the well-known *central limit theorem* [10].

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