Quantum transport and the Wigner distribution function for Bloch electrons in spatially homogeneous electric and magnetic fields

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The theory of Bloch electron dynamics for carriers in homogeneous electric and magnetic fields of arbitrary time dependence is developed in the framework of the Liouville equation. The Wigner distribution function (WDF) is determined from the single-particle density matrix in the ballistic regime, i.e., collision effects are excluded. In the theory, the single-particle transport equation is established with the electric field described in the vector potential gauge, and the magnetic field is treated in the symmetric gauge. No specific assumptions are made concerning the form of the initial distribution in momentum or configuration space. The general approach is to employ the accelerated Bloch state representation (ABR) as a basis so that the dependence upon the electric field, including multiband Zener tunneling, is treated exactly. Further, in the formulation of the WDF, we transform to a new set of variables so that the final WDF is gauge invariant and is expressed explicitly in terms of the position, kinetic momentum, and time. The methodology for developing the WDF is illustrated by deriving the exact WDF equation for free electrons in homogeneous electric and magnetic fields resulting in the same form as given by the collisionless Boltzmann transport equation (BTE). The methodology is then extended to the case of electrons described by an effective Hamiltonian corresponding to an arbitrary energy band function; the exact WDF equation results for the effective Hamiltonian case are shown to approximate the free electron results when taken to second order in the magnetic field. As a corollary, in these cases, it is shown that if the WDF is a wave packet, then the time rate of change of the electron quasimomentum is given by the Lorentz force. In treating the problem of Bloch electrons in a periodic potential in the presence of homogeneous electric and magnetic fields, the methodology for deriving the WDF reveals a multiband character due to the inherent nature of the Bloch states. The $\mathbf{K}_0$ *representation* of the Bloch envelope functions is employed to express the multiband WDF in a useful form. In examining the single-band WDF, it is found that the collisionless WDF equation matches the equivalent BTE to first order in the magnetic field. These results are necessarily extended to second order in the magnetic field by employing a unitary transformation that diagonalizes the Hamiltonian using the ABR to second order. The unitary transformation process includes a discussion of the multiband WDF transport analysis and the identification of the combined Zener-magnetic-field induced tunneling.

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I. INTRODUCTION

A central problem in the theory of solids is the question of how to construct the correct quantum-mechanical transport equation for charge carriers under the influence of both electric $\mathbf{E}$ and magnetic $\mathbf{B}$ fields. The first attempt at doing so was provided by Bloch in his fundamental paper [1] on the application of the quantum theory to transport phenomena. Bloch showed that electrons moving in solids could be treated as quasiparticles having an altered energy-momentum relation, $\varepsilon(\mathbf{k})$, different from the usual free-electron dispersion relation. The corresponding velocity of the electron wave packet constructed from a superposition of states from a single band centered at wave vector $\mathbf{k}$ is given by

$$\mathbf{v}(\mathbf{k}) = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k}), \tag{1}$$

which reduces to the usual expression for the velocity in the free-electron limit. Bloch then argued that the correct transport equation is the Boltzmann transport equation (BTE) where $\mathbf{v}$ is given by Eq. (1) and the scattering rates are calculated quantum mechanically using Fermi's *golden rule* of time-dependent perturbation theory. Thus the BTE for the single-particle distribution function should be written as

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \hbar^{-1}\mathbf{F}_L\cdot\nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t}\right)_c, \tag{2}$$

where $\mathbf{F}_L$ is given by the Lorentz force

$$\mathbf{F}_L = e\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right) \tag{3}$$

and $\mathbf{v}$ is given in Eq. (1); also, e is the electron charge, c is the speed of light, $\hbar$ is the reduced Planck constant, t is the time, $\mathbf{x}$ is the position vector, and $(\partial f/\partial t)_c$ represents the collision integral. Equation (2) has been very successful in providing the basic theoretical framework for analyzing low-field galvanomagnetic effects in semiconductors [2], although

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its justification is based only on quasiclassical considerations, i.e., it is not directly derived from the fundamental equations of quantum mechanics, but rather from the employment of classical dynamics applied to electron quasiparticles.

Nearly three decades after Bloch's seminal work, the quantum-mechanical derivation of Eq. (2) from the Liouville equation for the density matrix was given by Kohn and Luttinger [3] for electrons scattered by impurities in a weak uniform electric field; this work was later extended to the case of phonon scattering [4]. This density matrix approach was generalized to higher electric fields by Levinson [5] and by Barker [6], using the effective-mass approximation with the resulting inclusion of the intracollisional field effect. Subsequently, Krieger and Iafrate [7] have extended the previous results of Levinson [5] and Calecki and Pottier [8] to the multiband case for arbitrary electron energy dispersion relations including the effects of Zener tunneling, and demonstrated that the scattering matrix elements entering the collision term are both field and time dependent.

The formal justification of Eq. (2) for nonzero magnetic field has not been so straightforward. It is well known that even for free electrons, the electron energy eigenvalues are quantized in steps of $\hbar\omega_c$ (Landau levels) where $\omega_c = eB/mc$ is the electron cyclotron frequency. Also, in the high-field limit, i.e., $\hbar\omega_c \gg k_B T$ (k_B is the Boltzmann constant, T is ambient temperature), the electron distribution function can be expected to change significantly from one quantum level to the next with experimentally detectable consequences. This is the well-known origin of the de Haas-van Alphen oscillations in the magnetic susceptibility of metals in zero electric fields. In an effort to take into account the existence of quantizing magnetic fields in the transport phenomena for free electrons, Adams and Holstein [9] employed as a basis the harmonic oscillator states corresponding to Landau levels. They then showed how the current could be calculated from the Liouville equation in this representation. This formulation significantly departs from the quasiclassical description given by Eq. (2) in that the current depends on the off-diagonal elements of the density matrix.

Rhetorically, the questions arise as to whether Eq. (2) is valid for relatively high magnetic fields, and, further, is it possible to derive a transport equation for a quantum distribution function which is defined within a classical phase space picture. In zero magnetic field, Krieger, Kiselev, and Iafrate [10] made use of the effective Hamiltonian to derive the Wigner distribution function (WDF) equation for a random distribution of impurities. However, if one wants to go beyond an effective Hamiltonian approach for Bloch electron dynamics in the electric and magnetic fields so that both interband tunneling and the proper field- and time-dependent scattering matrix elements may be included as previously done by Krieger and Iafrate [7] for the case of electric field alone, then a description in terms of a classical phase space WDF approach would be desirable since the exact solution to the Schrödinger equation for a Bloch electron in electric and magnetic fields is not known. Therefore we are motivated [11] to address this subject.

In this paper, the theory of Bloch electron transport in homogeneous electric and magnetic fields of arbitrary time dependence is developed within the framework of the Liouville equation. The phase space WDF is determined from the single-particle density matrix within the ballistic regime, i.e., collision effects are excluded, although the methodology for including such effects is straightforward. The electric field is treated in the vector potential gauge and the magnetic field is described in the symmetric gauge. No specific assumptions are adopted concerning the form of the initial distribution in momentum or configuration space. The general approach is to utilize the accelerated Bloch state representation (ABR) as a basis so that the dependence upon the electric field, including the multiband Zener tunneling, is treated exactly. In the formulation of the WDF, we transform to a set of variables based on position, kinetic momentum, and time to ensure the gauge invariance of the WDF in our problem.

In Sec. II, the methodology for developing the WDF is described and illustrated by deriving the exact WDF equation for free electrons in homogeneous electric and magnetic fields resulting in the same form as given by the collisionless BTE. In Sec. III, the methodology is extended to the case of electrons described by an effective Hamiltonian corresponding to an arbitrary energy-band function. The exact equation for the WDF is obtained in this case and is shown to approximate the free-electron results when taken to second order in the magnetic field. As a corollary, it is shown that if the WDF of Secs. II and III is a wave packet, then the time rate of change of the electron quasimomentum is given by the Lorentz force. In Sec. IV, the problem of Bloch electrons in a crystal potential in the presence of electric and magnetic fields is treated. The methodology for deriving the WDF reveals a multiband structure due to the inherent nature of the Bloch states. Use is made of the so-called "$\mathbf{K}_0$ representation″ outlined in Appendix A to express the multiband WDF in a user friendly form. In order to obtain results beyond first order in the magnetic field, it is necessary to employ a unitary transformation that diagonalizes the Hamiltonian using the ABR to second order in the magnetic field. The unitary transformation process results in an analysis for the single-band WDF equation and a discussion of multiband transport properties leading to the identification of a combined Zener magnetic field induced tunneling. Results also include the explicit development of the multiband WDF to first order in $(\mathbf{K} - \mathbf{K}_0)$.

II. DYNAMICS OF FREE ELECTRONS IN HOMOGENEOUS ELECTRIC AND MAGNETIC FIELDS

It has been established previously [7] that given an arbitrary initial distribution at $t = t_0$, when the fields are turned on, the equation for the density matrix operator $\hat{f}(t)$ may be written as

$$i\hbar\frac{\partial \hat{f}}{\partial t} - [\hat{H},\hat{f}] = C_s\{\hat{f}(t)\}, \tag{4}$$

where $C_s\{\hat{f}(t)\}$ involves the scattering Hamiltonian and $\hat{H}$ is the Hamiltonian in the absence of scattering. Equation (4) was first derived by Levinson [5] for the case in which electrons initially in thermal equilibrium are interacting with phonons. Our extension [7] of his result permits the use of Eq. (4) even for initial *nonequilibrium distributions and multiband dynamics*.

For free electrons interacting with spatially homogeneous but arbitrarily time-dependent electric and magnetic fields the

Hamiltonian is

$$\hat{H} = \frac{1}{2m}\Big[\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\Big]^2, \tag{5}$$

where m is the free-electron mass and $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{x}}$ is the operator of the electron momentum $\mathbf{p}$. The vector potential $\mathbf{A}(\mathbf{x},t)$ includes the homogeneous but arbitrarily time-dependent external electric and magnetic field contributions as

$$\mathbf{A}(\mathbf{x},t) = \mathbf{A}_1(t) + \mathbf{A}_2(\mathbf{x},t), \tag{6}$$

with

$$\mathbf{A}_1(t) = -c\int_0^t \mathbf{E}(t')dt' \tag{7a}$$

and

$$\mathbf{A}_2(\mathbf{x},t) = \tfrac{1}{2}\mathbf{B}(t)\times\mathbf{x}. \tag{7b}$$

Consistent with Maxwell's equations, we find that Eq. (6) yields

$$-\frac{1}{c}\frac{\partial\mathbf{A}(\mathbf{x},t)}{\partial t} = \mathbf{E}(t) - \frac{1}{2c}\dot{\mathbf{B}}(t)\times\mathbf{x} \equiv \boldsymbol{\mathcal{E}}(\mathbf{x},t) \tag{8a}$$

and

$$\nabla_{\mathbf{x}}\times\mathbf{A}(\mathbf{x},t) = \mathbf{B}(t). \tag{8b}$$

In $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ of Eq. (8a), the first term is the external electric field, and the second term is the induced electric field resulting from Faraday's law; if $\mathbf{B}(t)$ were assumed to be constant, then the induced term would be non-existent and $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ reduces to $\mathbf{E}(t)$ alone. Note that taking the "*curl*" of $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ in Eq. (8a) results in

$$\nabla_{\mathbf{x}}\times\boldsymbol{\mathcal{E}} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t},$$

so that the vector potential of Eq. (6) yields the Maxwell equation for Faraday's law.

In using Eqs. (5) and (6) and expanding the kinetic term while noting that $\hat{\mathbf{p}}$ and $\mathbf{A}_2$ commute, we see that

$$\hat{H} = \hat{H}_0 - \frac{e}{mc}\mathbf{A}_2\cdot\Big(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_1\Big) + \frac{e^2}{2mc^2}\mathbf{A}_2^2 \equiv \hat{H}_0 + V_1 + V_2, \tag{9}$$

where the Hamiltonian

$$\hat{H}_0 = \frac{1}{2m}\Big[\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_1(t)\Big]^2 \tag{10}$$

describes the free electron in the external electric field alone, and the next two terms in Eq. (9), V_1 and V_2, are first and second order in the magnetic field.

To adopt an appropriate basis set with which to evaluate Eq. (4), we see in Eqs. (9) and (10) that a natural basis to proceed would be the accelerated state representation which are the instantaneous eigenstates of $\hat{H}_0$ in Eq. (10). As such, the accelerated states are

$$\psi_{\mathbf{K}}(\mathbf{x}) = \Omega^{-1/2}e^{i\mathbf{K}\cdot\mathbf{x}} \equiv |\mathbf{K}\rangle, \tag{11a}$$

with eigenvalues $\varepsilon^0(\mathbf{k}(t)) = \hbar^2\mathrm{k}^2(t)/2m$, and where $\mathbf{k}(t)$ is the time-dependent wave vector due to acceleration by the electric field,

$$\mathbf{k}(t) = \mathbf{K} - \frac{e}{\hbar c}\mathbf{A}_1(t) \equiv \mathbf{K} + \mathbf{k}_c(t), \tag{11b}$$

with $\mathbf{k}_c(t) = (e/\hbar)\int_0^t \mathbf{E}(t')dt'$. Here, Ω is the normalization volume, $\mathrm{k} = |\mathbf{k}|$, and $\mathbf{K}$ is chosen such that $\psi_{\mathbf{K}}(\mathbf{x})$ satisfies periodic boundary conditions. It is noted that the choice of $|\mathbf{K}\rangle$ as a basis allows us to work in a representation in which the electron motion is indexed by the momentum $\mathbf{p} = \hbar\mathbf{K}$; if we had chosen to work in the representation based on the instantaneous eigenstates of the full Hamiltonian in Eq. (5), we would then have oscillator states which are inconvenient in that they are not eigenfunctions of the momentum operator.

In obtaining the WDF for the density matrix, we note that the WDF, $f(\mathbf{x},\mathbf{p})$, is fundamentally defined [12] as the off-diagonal matrix elements of the density matrix operator, $\hat{f}(t)$, in Eq. (4). As such,

$$f(\mathbf{x},\mathbf{p}) = (2\pi\hbar)^{-3}\int d\mathbf{y}\langle\mathbf{x}-\mathbf{y}/2|\hat{f}|\mathbf{x}+\mathbf{y}/2\rangle e^{i\mathbf{p}\cdot\mathbf{y}/\hbar}. \tag{12}$$

Then, for the complete set of basis states defined in Eq. (11a), we see that Eq. (12) can be expressed as

$$f(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{K}_1\mathbf{K}_2}\langle\mathbf{K}_1|\hat{f}|\mathbf{K}_2\rangle(2\pi\hbar)^{-3}\int d\mathbf{y}\psi^*_{\mathbf{K}_2}(\mathbf{x}+\mathbf{y}/2) \times \psi_{\mathbf{K}_1}(\mathbf{x}-\mathbf{y}/2)e^{i\mathbf{p}\cdot\mathbf{y}/\hbar}. \tag{13}$$

Using the explicit spectral dependence for $\psi_{\mathbf{K}}(\mathbf{x})$ in the integral over $\mathbf{y}$ of Eq. (13), and utilizing $(2\pi\hbar)^{-3}\int d\mathbf{y}e^{i\mathbf{p}\cdot\mathbf{y}/\hbar} = \delta(\mathbf{p})$, we obtain

$$f(\mathbf{x},\mathbf{p}) = \Omega^{-1}\sum_{\mathbf{K}_1\mathbf{K}_2}e^{i(\mathbf{K}_1-\mathbf{K}_2)\cdot\mathbf{x}}\langle\mathbf{K}_1|\hat{f}|\mathbf{K}_2\rangle \times \delta[\mathbf{p}-\hbar(\mathbf{K}_1+\mathbf{K}_2)/2]. \tag{14}$$

Letting

$$\mathbf{K}_1 = \mathbf{K} + \frac{\mathbf{u}}{2}, \quad \mathbf{K}_2 = \mathbf{K} - \frac{\mathbf{u}}{2} \tag{15}$$

in Eq. (14), the WDF becomes

$$f(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{K}} f^0(\mathbf{x},\mathbf{K})\delta(\mathbf{p}-\hbar\mathbf{K}) = f^0(\mathbf{x},\mathbf{K})|_{\mathbf{p}=\hbar\mathbf{K}}, \tag{16a}$$

where

$$f^0(\mathbf{x},\mathbf{K}) = \Omega^{-1}\sum_{\mathbf{u}}\Big\langle\mathbf{K}+\frac{\mathbf{u}}{2}\Big|\hat{f}\Big|\mathbf{K}-\frac{\mathbf{u}}{2}\Big\rangle e^{i\mathbf{u}\cdot\mathbf{x}}; \tag{16b}$$

here, $\mathbf{p} = \hbar\mathbf{K}$, and $\langle\mathbf{K}_1|\hat{f}|\mathbf{K}_2\rangle$ are the momentum matrix elements of the density matrix operator in Eq. (4) evaluated at $\mathbf{K}_1,\mathbf{K}_2$ of Eq. (15). Finally, in Eq. (16b), we make the change of variables [13]

$$\boldsymbol{k}(\mathbf{x},t) = \mathbf{K} - \frac{e}{\hbar c}\mathbf{A}(\mathbf{x},t), \tag{17}$$

where the Jacobian of the transformation from $\boldsymbol{k}$ to $\mathbf{K}$ is unity, and where $\hbar\boldsymbol{k}(\mathbf{x},t)$ is the $(\mathbf{x}$,t)-dependent kinetic momentum; then we obtain

$$F(\mathbf{x},\boldsymbol{k},t) \equiv f(\mathbf{x},\mathbf{K},t), \tag{18}$$

the gauge invariant WDF [5,13] in the $\boldsymbol{k}$ representation for an electron subjected to the vector potential $\mathbf{A}(\mathbf{x},t)$ of Eq. (6).

For the Hamiltonian of Eq. (9), we determine the equation of motion for the WDF as outlined in Eqs. (13)–(18) considering, for simplicity, the case of ballistic or collisionless transport for which $C_s\{\hat{f}\} \equiv 0$ in Eq. (4). Then, we basically start with

$$i\hbar\langle \mathbf{K}_1|\frac{\partial \hat{f}}{\partial t}|\mathbf{K}_2\rangle = \langle \mathbf{K}_1|[\hat{H},\hat{f}]|\mathbf{K}_2\rangle. \tag{19}$$

Since $|\mathbf{K}\rangle$ is independent of time, we note that $\langle \mathbf{K}_1|\partial \hat{f}/\partial t|\mathbf{K}_2\rangle = \partial\langle \mathbf{K}_1|\hat{f}|\mathbf{K}_2\rangle/\partial t$; as well the Hamiltonian in Eq. (9) is reexpressed as

$$\hat{H} = \hat{H}_0 - \frac{e}{2mc}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_1\right)\cdot(\mathbf{B}\times\mathbf{x}) + \frac{e^2}{8mc^2}(\mathbf{B}\times\mathbf{x})^2. \tag{20}$$

Using the vector identity $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}$ in the second term, we can write

$$\hat{H} = \hat{H}_0 - \frac{e}{2mc}\left[\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_1\right)\times\mathbf{B}\right]\cdot\mathbf{x} + \frac{e^2}{8mc^2}(\mathbf{B}\times\mathbf{x})^2. \tag{21}$$

Noting that $(\hat{\mathbf{p}} - (e/c)\mathbf{A}_1)|\mathbf{K}\rangle = (\hbar\mathbf{K} - (e/c)\mathbf{A}_1)|\mathbf{K}\rangle$ and $\mathbf{x}|\mathbf{K}\rangle = \frac{1}{i}\nabla_{\mathbf{K}}|\mathbf{K}\rangle$, we obtain the term on the right-hand side of Eq. (19) as

$$\langle \mathbf{K}_1|[\hat{H},\hat{f}]|\mathbf{K}_2\rangle = [\varepsilon_+(\mathbf{K}_1) - \varepsilon_-(\mathbf{K}_2)]f(\mathbf{K}_1,\mathbf{K}_2,t), \tag{22}$$

where

$$\varepsilon(\mathbf{K})_\pm = \frac{1}{2m}\left\{\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1\right)^2 \pm \frac{e}{c}\left[\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1\right)\times\mathbf{B}\right]\cdot\frac{1}{i}\nabla_{\mathbf{K}} + \frac{e^2}{4c^2}\left(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}}\right)^2\right\}$$

and $f(\mathbf{K}_1,\mathbf{K}_2,t) \equiv \langle \mathbf{K}_1|\hat{f}(t)|\mathbf{K}_2\rangle$.

Next, we change the variables as prescribed by Eq. (15) while noting that

$$\nabla_{\mathbf{K}_1} f(\mathbf{K}_1,\mathbf{K}_2,t) = \left(\frac{1}{2}\nabla_{\mathbf{K}} + \nabla_{\mathbf{u}}\right) f\left(\mathbf{K} + \frac{\mathbf{u}}{2},\mathbf{K} - \frac{\mathbf{u}}{2},t\right),$$
$$\nabla_{\mathbf{K}_2} f(\mathbf{K}_1,\mathbf{K}_2,t) = \left(\frac{1}{2}\nabla_{\mathbf{K}} - \nabla_{\mathbf{u}}\right) f\left(\mathbf{K} + \frac{\mathbf{u}}{2},\mathbf{K} - \frac{\mathbf{u}}{2},t\right). \tag{23}$$

Thus, using (15) and (23), Eq. (22) becomes

$$\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\right|[\hat{H},\hat{f}]\left|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle = \frac{1}{m}\left\{\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1\right)\cdot\hbar\mathbf{u} + \frac{e}{2c}\left[\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1\right)\times\mathbf{B}\right]\cdot\frac{1}{i}\nabla_{\mathbf{K}} + \frac{e}{2c}(\hbar\mathbf{u}\times\mathbf{B})\cdot\frac{1}{i}\nabla_{\mathbf{u}} + \frac{e^2}{4c^2}\left(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}}\right)\cdot\left(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{u}}\right)\right\} f\left(\mathbf{K} + \frac{\mathbf{u}}{2},\mathbf{K} - \frac{\mathbf{u}}{2},t\right). \tag{24}$$

Noting that $(\mathbf{B}\times\nabla_{\mathbf{K}})\cdot(\mathbf{B}\times\nabla_{\mathbf{u}}) = [(\mathbf{B}\times\nabla_{\mathbf{u}})\times\mathbf{B}]\cdot\nabla_{\mathbf{K}}$ and $(\mathbf{u}\times\mathbf{B})\cdot\nabla_{\mathbf{u}} = \mathbf{u}\cdot(\mathbf{B}\times\nabla_{\mathbf{u}})$, then Eq. (24) becomes

$$\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\right|[\hat{H},\hat{f}]\left|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle = \frac{1}{m}\left\{\hbar\mathbf{u}\cdot\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1 + \frac{e}{2c}\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{u}}\right) + \frac{e}{2c}\left[\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}_1 + \frac{e}{2c}\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{u}}\right)\times\mathbf{B}\right]\cdot\frac{1}{i}\nabla_{\mathbf{K}}\right\} \times f\left(\mathbf{K} + \frac{\mathbf{u}}{2},\mathbf{K} - \frac{\mathbf{u}}{2},t\right). \tag{25}$$

In following the definition of the WDF in (16a) and (16b), we multiply Eq. (25) by $e^{i\mathbf{u}\cdot\mathbf{x}}/\Omega$ and sum over $\mathbf{u}$; we then integrate the $\nabla_{\mathbf{u}}$ term by parts, noting that $\sum_{\mathbf{u}} e^{i\mathbf{u}\cdot\mathbf{x}} i\nabla_{\mathbf{u}} f(\mathbf{K},\mathbf{u},t) = \sum_{\mathbf{u}} \mathbf{x}e^{i\mathbf{u}\cdot\mathbf{x}} f(\mathbf{K},\mathbf{u},t)$ where the surface term goes to zero as $\mathbf{u}$ tends to infinity; we also use $\mathbf{u}e^{i\mathbf{u}\cdot\mathbf{x}} = -i\nabla_{\mathbf{x}} e^{i\mathbf{u}\cdot\mathbf{x}}$ and $\nabla_{\mathbf{x}}\cdot(\mathbf{B}\times\mathbf{x}) = 0$ to obtain for Eq. (25),

$$\Omega^{-1}\sum_{\mathbf{u}}\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\right|[\hat{H},\hat{f}]\left|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}} = \frac{\hbar}{m}\left[\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]\cdot\frac{1}{i}\nabla_{\mathbf{x}} f(\mathbf{x},\mathbf{K},t) + \left\{\frac{e}{2mc}\left[\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]\times\mathbf{B}\right\}\cdot\frac{1}{i}\nabla_{\mathbf{K}} f(\mathbf{x},\mathbf{K},t). \tag{26}$$

For $i\hbar(\partial\hat{f}/\partial t)$ in Eq. (4), we obtain, using (16a), that

$$\Omega^{-1}\sum_{\mathbf{u}} i\hbar\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\right|\frac{\partial\hat{f}}{\partial t}\left|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}} = i\hbar\frac{\partial f(\mathbf{x},\mathbf{K},t)}{\partial t}. \tag{27}$$

Thus the WDF in variables $(\mathbf{x},\mathbf{K},t)$ is determined by the equation

$$\Omega^{-1}\sum_{\mathbf{u}}\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\right| i\hbar\frac{\partial\hat{f}}{\partial t} - [\hat{H},\hat{f}]\left|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}} \equiv i\hbar\left\{\frac{\partial}{\partial t} + \frac{1}{m}\left[\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]\cdot\nabla_{\mathbf{x}} + \frac{e}{2\hbar mc}\left[\left(\hbar\mathbf{K} - \frac{e}{c}\mathbf{A}(\mathbf{x},t)\right)\times\mathbf{B}\right]\cdot\nabla_{\mathbf{K}}\right\} f(\mathbf{x},\mathbf{K},t) = 0. \tag{28}$$

Lastly, we change variables in Eq. (28) as noted in (17) and (18) and use the following transformation properties:

$$\frac{\partial f}{\partial t} = \frac{\partial F}{\partial t} + \nabla_{\boldsymbol{k}} F \cdot \dot{\boldsymbol{k}} = \frac{\partial F}{\partial t} + \hbar^{-1} e \boldsymbol{\mathcal{E}}(\mathbf{x},t) \cdot \nabla_{\boldsymbol{k}} F, \quad (29a)$$

$$\nabla_{\mathbf{K}} f(\mathbf{x},\mathbf{K},t) = \nabla_{\boldsymbol{k}} F(\mathbf{x},\boldsymbol{k},t), \quad (29b)$$

and

$$\nabla_{x_i} f = \nabla_{x_i} F + \frac{\partial F}{\partial \boldsymbol{k}} \cdot \frac{\partial \boldsymbol{k}}{\partial x_i} = \nabla_{x_i} F + \frac{e}{2\hbar c}(\mathbf{B} \times \nabla_{\boldsymbol{k}} F)_i. \quad (29c)$$

Therefore the equation for the WDF from Eq. (28) becomes

$$\frac{\partial}{\partial t} F(\mathbf{x},\boldsymbol{k},t) + \mathbf{v}(\boldsymbol{k}) \cdot \nabla_{\mathbf{x}} F(\mathbf{x},\boldsymbol{k},t) + \hbar^{-1}\left[e\boldsymbol{\mathcal{E}}(\mathbf{x},t) + \frac{e}{c}\mathbf{v}(\boldsymbol{k}) \times \mathbf{B}\right] \cdot \nabla_{\boldsymbol{k}} F(\mathbf{x},\boldsymbol{k},t) = 0, \quad (30)$$

where $\mathbf{v}(\boldsymbol{k}) = \hbar\boldsymbol{k}/m$ and $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ is given in Eq. (8a). Equation (30) for $F(\mathbf{x},\boldsymbol{k},t)$ is the exact equation for the collisionless WDF obtained with the Hamiltonian of Eq. (9); it is also the identical form of the collisionless BTE for the same problem. We also note here that the change of variables from $\mathbf{K}$ to $\boldsymbol{k}(\mathbf{x},t) = \mathbf{K} - (e/\hbar c)\mathbf{A}(\mathbf{x},t)$ has introduced the total $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ from Eq. (8a) into the gauge invariant form of the WDF through the transformations of Eq. (29a).

For simplicity in our continued analysis, we hereafter consider $\mathbf{B}$ to be a constant so that the $\dot{\mathbf{B}}(t)$ term vanishes in Eq. (8a) and thus $\boldsymbol{\mathcal{E}}(\mathbf{x},t) \equiv \mathbf{E}(t)$, the external electric field alone. However, if we had chosen to assume that $\mathbf{B}$ were time dependent, then $\mathbf{E}(t)$ would have to be replaced by $\boldsymbol{\mathcal{E}}(\mathbf{x},t)$ in the final results in accordance with Eq. (29a).

We point out that Levinson [5] asserts Eq. (30) [for $\mathbf{B}$ constant and therefore $\boldsymbol{\mathcal{E}} = \mathbf{E}(t)$] without proof. He also only considers the case in which the system is initially in thermal equilibrium, and under such conditions, the WDF is a function of $(\boldsymbol{k},t)$ alone so that the term $\mathbf{v} \cdot \nabla_{\mathbf{x}} F(\mathbf{x},\boldsymbol{k},t)$ in Eq. (30) is missing. In our derivation, the initial condition $F(\mathbf{x},\boldsymbol{k},t = t_0)$ is completely arbitrary for an admissible Wigner distribution function, so we can discuss the motion of wave packets in the presence of arbitrarily large electric and magnetic fields in the absence of collisions. This follows if one multiplies Eq. (30) [with $\mathbf{B}$ assumed to be constant so that $\boldsymbol{\mathcal{E}} = \mathbf{E}(t)$] by $k_i(t)$, the ith component of $\boldsymbol{k}(t)$, and integrate by parts to get

$$\frac{d}{dt}\langle \hbar k_i \rangle = \int \left(e\mathbf{E} + \frac{e}{c}\mathbf{v} \times \mathbf{B}\right)_i F(\mathbf{x},\boldsymbol{k},t) d\mathbf{x} d\boldsymbol{k}, \quad (31)$$

where

$$\langle \hbar k_i \rangle = \hbar \int k_i F(\mathbf{x},\boldsymbol{k},t) d\mathbf{x} d\boldsymbol{k}.$$

Thus, if the function

$$F(\boldsymbol{k},t) = \int F(\mathbf{x},\boldsymbol{k},t) d\mathbf{x}$$

is peaked about some $\boldsymbol{k}(t)$, then it follows from $\langle \hbar k_i \rangle$ that

$$\hbar \frac{d}{dt}\boldsymbol{k}(t) = e\mathbf{E}(t) + \frac{e}{c}\mathbf{v}(\boldsymbol{k}(t)) \times \mathbf{B} \quad (32)$$

for arbitrary strengths of $\mathbf{E}$ and $\mathbf{B}$. Thus not only is the classical phase space description possible, but the results are exactly the same as those given by the quasiclassical approach. However, unlike the Boltzmann distribution function, the WDF, $F(\mathbf{x},\boldsymbol{k},t)$, need not be positive everywhere; its exact structure depends on the initial conditions, and $F(\mathbf{x},\boldsymbol{k},t)$ may be negative in certain regions of configuration and momentum space due to quantum effects.

III. EXTENSION TO ELECTRONS IN SOLIDS DESCRIBED BY AN EFFECTIVE HAMILTONIAN

We now proceed as described in Sec. II, except here the Hamiltonian of Eq. (5) is replaced by the effective Hamiltonian

$$\hat{H} = \varepsilon([\hat{\mathbf{p}} - (e/c)\mathbf{A}(\mathbf{x},t)]/\hbar), \quad (33)$$

and the zero magnetic field Hamiltonian is replaced by

$$\hat{H}_0 = \varepsilon([\hat{\mathbf{p}} - (e/c)\mathbf{A}_1(t)]/\hbar). \quad (34)$$

Here, it is assumed that $\varepsilon(\mathbf{K})$ is a physical single energy band and therefore $\hat{H}$ comes from a properly symmetrized Hermitian operator. We once again make use of the instantaneous eigenstates $|\mathbf{K}\rangle$ of $\hat{H}_0$ given by

$$\hat{H}_0|\mathbf{K}\rangle = \varepsilon(\mathbf{K} - (e/\hbar c)\mathbf{A}_1(t))|\mathbf{K}\rangle, \quad (35)$$

with eigenvalues $\varepsilon(\mathbf{K} - (e/\hbar c)\mathbf{A}_1(t))$, which are still given by $|\mathbf{K}\rangle$ of Eq. (11a); they also satisfy the properties $\hat{\mathbf{p}}|\mathbf{K}\rangle = \hbar\mathbf{K}|\mathbf{K}\rangle$ and $\frac{1}{i}\nabla_{\mathbf{K}}|\mathbf{K}\rangle = \mathbf{x}|\mathbf{K}\rangle$ so that $\mathbf{A}(\mathbf{x},t)|\mathbf{K}\rangle = \mathbf{A}(\frac{1}{i}\nabla_{\mathbf{K}},t)|\mathbf{K}\rangle$. Thus, following the previous prescription for calculating the WDF from Eq. (19) for $\hat{H}$ in Eq. (33), we have

$$\langle \mathbf{K}_1|[\hat{H},\hat{f}]|\mathbf{K}_2\rangle f(\mathbf{K}_1,\mathbf{K}_2,t) = [\varepsilon_+(\mathbf{K}_1) - \varepsilon_-(\mathbf{K}_2)] f(\mathbf{K}_1,\mathbf{K}_2,t), \quad (36)$$

where

$$\varepsilon_\pm(\mathbf{K}) = \varepsilon\left[\mathbf{K} + \mathbf{k}_c(t) \pm \frac{e}{2\hbar c}\left(\mathbf{B} \times \frac{1}{i}\nabla_{\mathbf{K}}\right)\right]$$

and $\mathbf{k}_c(t)$ is defined in Eq. (11b). Changing variables from $\mathbf{K}_{1,2}$ to $\mathbf{K} \pm \mathbf{u}/2$ and using (23), we obtain

$$\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}\middle|[\hat{H},\hat{f}]\middle|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle = \left[\varepsilon_+\left(\mathbf{K} + \frac{\mathbf{u}}{2}\right) - \varepsilon_-\left(\mathbf{K} - \frac{\mathbf{u}}{2}\right)\right] \times f\left(\mathbf{K} + \frac{\mathbf{u}}{2},\mathbf{K} - \frac{\mathbf{u}}{2},t\right), \quad (37a)$$

where

$$\varepsilon_\pm\left(\mathbf{K} \pm \frac{\mathbf{u}}{2}\right) = \varepsilon\left[\mathbf{K} \pm \frac{\mathbf{u}}{2} + \mathbf{k}_c(t) \pm \frac{e}{2\hbar c}\mathbf{B} \times \frac{1}{i}\left(\frac{1}{2}\nabla_{\mathbf{K}} \pm \nabla_{\mathbf{u}}\right)\right].$$

We multiply Eq. (37a) by $e^{i\mathbf{u}\cdot\mathbf{x}}/\Omega$ and sum over $\mathbf{u}$; then using the relation $\mathbf{u}e^{i\mathbf{u}\cdot\mathbf{x}} = \frac{1}{i}\nabla_{\mathbf{x}} e^{i\mathbf{u}\cdot\mathbf{x}}$ and integrating over $\mathbf{u}$ by parts, we obtain

$$\Omega^{-1}\sum_{\mathbf{u}} e^{i\mathbf{u}\cdot\mathbf{x}}\left\langle \mathbf{K} + \frac{\mathbf{u}}{2}|[\hat{H},\hat{f}]|\mathbf{K} - \frac{\mathbf{u}}{2}\right\rangle = \left\{\varepsilon\left[\mathbf{K} - \frac{e}{\hbar c}\mathbf{A} + \frac{1}{2i}\left(\nabla_{\mathbf{x}} + \frac{e}{2\hbar c}\mathbf{B} \times \nabla_{\mathbf{K}}\right)\right] - \varepsilon\left[\mathbf{K} - \frac{e}{\hbar c}\mathbf{A} - \frac{1}{2i}\left(\nabla_{\mathbf{x}} + \frac{e}{2\hbar c}\mathbf{B} \times \nabla_{\mathbf{K}}\right)\right]\right\} f(\mathbf{x},\mathbf{K},t). \quad (37b)$$

Again, changing variables to $\boldsymbol{k}$ and $F(\mathbf{x},\boldsymbol{k},t)$ as in Eqs. (17) and (18) and using the relations (29a)–(29c), we get

$$\Omega^{-1}\sum_{\mathbf{u}} e^{i\mathbf{u}\cdot\mathbf{x}}\left\langle \mathbf{K}+\frac{\mathbf{u}}{2}\right|[\hat{H},\hat{f}]\left|\mathbf{K}-\frac{\mathbf{u}}{2}\right\rangle = \{\varepsilon(\boldsymbol{k}+\mathbf{q})-\varepsilon(\boldsymbol{k}-\mathbf{q})\}F(\mathbf{x},\boldsymbol{k},t), \quad (38)$$

where $\mathbf{q}=\frac{1}{2i}(\nabla_{\mathbf{x}}+\frac{e}{\hbar c}\mathbf{B}\times\nabla_{\boldsymbol{k}})$ and $\nabla_{\mathbf{x}}$ commutes with $\nabla_{\boldsymbol{k}}$. Now, it follows from Eqs. (19) and (38) as well as from the use of Eq. (29a) that the equation for the WDF takes the form

$$i\hbar\left\{\frac{\partial}{\partial t}+\hbar^{-1}e\mathbf{E}(t)\cdot\nabla_{\boldsymbol{k}}\right\}F(\mathbf{x},\boldsymbol{k},t) = \{\varepsilon(\boldsymbol{k}+\mathbf{q})-\varepsilon(\boldsymbol{k}-\mathbf{q})\}F(\mathbf{x},\boldsymbol{k},t). \quad (39)$$

This is the *exact equation* for the collisionless quantum transport WDF for the effective Hamiltonian in homogeneous electric and magnetic fields. In noting that for a single band, the periodic function $\varepsilon(\boldsymbol{k})$ can be represented by the Fourier expansion

$$\varepsilon(\boldsymbol{k})=\sum_{\mathbf{l}}\varepsilon(\mathbf{l})\,e^{i\boldsymbol{k}\cdot\mathbf{l}},$$

so that $\varepsilon(k\pm\mathbf{q})$ becomes

$$\varepsilon(\boldsymbol{k}\pm\mathbf{q})=\sum_{\mathbf{l}}\varepsilon(\mathbf{l})\,e^{i(\boldsymbol{k}\pm\mathbf{q})\cdot\mathbf{l}};$$

we can then write the energy difference on the right-hand side of Eq. (39) as

$$\varepsilon(\boldsymbol{k}+\mathbf{q})-\varepsilon(\boldsymbol{k}-\mathbf{q}) = 2i\sum_{\mathbf{l}}\varepsilon(\mathbf{l})\,e^{i\boldsymbol{k}\cdot\mathbf{l}}\sin(\mathbf{q}\cdot\mathbf{l}) \simeq 2\hbar\mathbf{v}(\boldsymbol{k})\cdot\mathbf{q}+O(\mathbf{q}^3), \quad (40)$$

where $\mathbf{v}(\boldsymbol{k})=\hbar^{-1}\nabla_{\boldsymbol{k}}\varepsilon(\boldsymbol{k})$. Making use of (40) in (39) results in

$$\left\{\frac{\partial}{\partial t}+\hbar^{-1}e\mathbf{E}(t)\cdot\nabla_{\boldsymbol{k}}\right\}F(\mathbf{x},\boldsymbol{k},t) = -\mathbf{v}(\boldsymbol{k})\cdot\left(\nabla_{\mathbf{x}}+\frac{e}{\hbar c}\mathbf{B}\times\nabla_{\boldsymbol{k}}\right)F(\mathbf{x},\boldsymbol{k},t)+O(\mathbf{B}^3).$$

Then to $O(\mathbf{B}^2)$, the equation to the WDF is found to be

$$\frac{\partial}{\partial t}F(\mathbf{x},\boldsymbol{k},t)+\mathbf{v}(\boldsymbol{k})\cdot\nabla_{\mathbf{x}}F(\mathbf{x},\boldsymbol{k},t) +\hbar^{-1}\left[e\mathbf{E}(t)+\frac{e}{c}(\mathbf{v}\times\mathbf{B})\right]\cdot\nabla_{\boldsymbol{k}}F(\mathbf{x},\boldsymbol{k},t)=0, \quad (41)$$

where we have used the relations $\mathbf{v}\cdot(\mathbf{B}\times\nabla_{\boldsymbol{k}})F=(\mathbf{v}\times\mathbf{B})\cdot\nabla_{\boldsymbol{k}}F$ and $(\mathbf{B}\times\nabla_{\boldsymbol{k}})\cdot\mathbf{v}=0$.

Equation (41) is the analog of Eq. (30) obtained for free electrons. The major difference between the two results is that for free electrons with $\mathbf{v}=\hbar\boldsymbol{k}/m$, the derived quantum transport equation for the WDF is *exact*, whereas for the general energy-band function $\varepsilon(\boldsymbol{k})$, the result is *approximate*, good to order $O(\mathbf{B}^2)$, and where $\mathbf{v}=\hbar^{-1}\nabla_{\boldsymbol{k}}\varepsilon(\boldsymbol{k})$. Also, in keeping with the discussion in Sec. II on the WDF as a wave packet, again with no scattering, the rate of change of the electron quasimomentum is given by the Lorentz force even to $O(\mathbf{B}^3)$, since the term of $O(\mathbf{B}^3)$ (if it is present) in Eq. (41) does not contribute to the $d\langle\hbar\boldsymbol{k}\rangle/dt$.

IV. BLOCH ELECTRONS IN HOMOGENEOUS ELECTRIC AND MAGNETIC FIELDS; SINGLE-BAND RESULTS AND MULTI-BAND CONSIDERATIONS

A. Development of multiband Wigner distribution function

For Bloch electrons interacting with spatially homogeneous, but arbitrarily time-dependent, electric and magnetic fields, the Hamiltonian is

$$\hat{H}=\frac{1}{2m}\left[\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A}(\mathbf{x},t)\right]^2+V_c(\mathbf{x}), \quad (42)$$

where $V_c(\mathbf{x})$ is the periodic potential of the crystal. The vector potential $\mathbf{A}(\mathbf{x},t)$ includes the electric and magnetic field contributions given in Eqs. (6)–(7b). Thus, as in Eq. (9), expanding the kinetic term while noting that $\hat{\mathbf{p}}$ and $\mathbf{A}_2$ commute, we arrive at

$$\hat{H}=\hat{H}_0-\frac{e}{mc}\mathbf{A}_2\cdot\left(\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A}_1\right)+\frac{e^2}{2mc^2}\mathbf{A}_2^2, \quad (43a)$$

where the Hamiltonian term

$$\hat{H}_0=\frac{1}{2m}\left[\hat{\mathbf{p}}-\frac{e}{c}\mathbf{A}_1(t)\right]^2+V_c(\mathbf{x}) \quad (43b)$$

describes the Bloch electron in the electric field alone, and the next two terms are first and second order in the magnetic field. [Here, we note that the energy shifts due to the two magnetic field terms are generally small compared to the $\hat{H}_0$ term for applicable laboratory field strengths; therefore, throughout this discourse, we consider only changes induced by the magnetic field to second order, although higher orders can be necessarily obtained with effort (see J. Callaway [20]).]

To adopt an appropriate basis set with which to evaluate Eq. (4), we see in Eqs. (43a) and (43b) that a natural basis with which to proceed here is the ABR, which are the instantaneous eigenstates of $\hat{H}_0$,

$$\psi_{n\mathbf{K}}(\mathbf{x},t)=\Omega^{-1/2}e^{i\mathbf{K}\cdot\mathbf{x}}u_{n\mathbf{k}(t)}(\mathbf{x})\equiv|n,\mathbf{K};t\rangle, \quad (44)$$

with instantaneous Bloch eigenvalues $\varepsilon_n^0(\mathbf{k}(t))=\varepsilon_{n\mathbf{k}}^0$ and $\mathbf{k}(t)$ defined in Eq. (11b). Following the WDF analysis from Eqs. (12)–(14), we insert the complete set of ABR states of Eq. (44) into Eq. (12) to obtain

$$f(\mathbf{x},\mathbf{p},t)=\sum_{n_1\mathbf{K}_1,n_2\mathbf{K}_2}\langle n_1,\mathbf{K}_1;t|\hat{f}|n_2,\mathbf{K}_2;t\rangle T_{n_2\mathbf{K}_2n_1\mathbf{K}_1}(\mathbf{x},\mathbf{p},t),$$

$$T_{n_2\mathbf{K}_2n_1\mathbf{K}_1}(\mathbf{x},\mathbf{p},t)=(2\pi\hbar)^{-3}\int d\mathbf{y}\psi^*_{n_2\mathbf{K}_2}\left(\mathbf{x}+\frac{\mathbf{y}}{2},t\right)\times\psi_{n_1\mathbf{K}_1}\left(\mathbf{x}-\frac{\mathbf{y}}{2},t\right)e^{i\mathbf{p}\cdot\mathbf{y}/\hbar}; \quad (45)$$

the $T_{n_2\mathbf{K}_2n_1\mathbf{K}_1}(\mathbf{x},\mathbf{p},t)$ are commonly referred to as the transition functions [14], and they form a complete orthonormal set in phase space. The general properties of $T_{n_2\mathbf{K}_2n_1\mathbf{K}_1}(\mathbf{x},\mathbf{p},t)$ are reviewed by Moyal [14]. The function $f(\mathbf{x},\mathbf{p},t)$ can be presented in the form of a multiband WDF [15]

$$f(\mathbf{x},\mathbf{p},t)=\sum_{n_1n_2}f_{n_1n_2}(\mathbf{x},\mathbf{p},t), \quad (46a)$$

where the multiband components are

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = \sum_{\mathbf{K}_1\mathbf{K}_2} \langle n_1,\mathbf{K}_1;t|\hat{f}|n_2,\mathbf{K}_2;t\rangle T_{n_2\mathbf{K}_2n_1\mathbf{K}_1}(\mathbf{x},\mathbf{p},t). \tag{46b}$$

Using the explicit form of Eq. (44) for $\psi_{n\mathbf{K}}$ and using $\mathbf{K}_{1,2}$ as defined in Eq. (15), the multiband components can be expressed in a form comparable to Eqs. (16a) and (16b) as

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = \Omega^{-1}\sum_{\mathbf{Ku}} e^{i\mathbf{u}\cdot\mathbf{x}}\left\langle n_1,\mathbf{K}+\frac{\mathbf{u}}{2};t|\hat{f}|n_2,\mathbf{K}-\frac{\mathbf{u}}{2};t\right\rangle \times I_{n_2n_1}(\mathbf{x},\mathbf{p};\mathbf{u},\mathbf{K},t), \tag{47a}$$

where

$$I_{n_2n_1}(\mathbf{x},\mathbf{p};\mathbf{u},\mathbf{K},t) = (2\pi\hbar)^{-3}\int d\mathbf{y}u^*_{n_2,\mathbf{k}(t)-\mathbf{u}/2}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right) \times u_{n_1,\mathbf{k}(t)+\mathbf{u}/2}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)e^{i(\mathbf{p}-\hbar\mathbf{K})\cdot\mathbf{y}/\hbar}. \tag{47b}$$

Unlike the WDF of previous cases discussed in Secs. II and III, namely, Eqs. (16a) and (16b), which were based on plane-wave instantaneous eigenstates, the WDF of Eq. (47a) is more complex in that it reflects the multiband character of the ABR, including the explicit time dependence contained in the cellular components of the Bloch wave functions. Therefore $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ of Eq. (47a) generally manifests its time dependence from both the matrix elements of $\hat{f}$ and $I_{n_2n_1}$ of Eq. (47b). It follows from Eq. (47a) that the time derivative of $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ will depend on the product derivative of $\langle n_1,\mathbf{K}+\mathbf{u}/2;t|\hat{f}|n_2,\mathbf{K}-\mathbf{u}/2;t\rangle$ and $I_{n_2n_1}$. The time evolution of the matrix elements of $\hat{f}$ is governed by the Liouville equation as discussed in Secs. II and III and will be continued further in this section; the derivative of $I_{n_2n_1}$ will depend upon the time derivatives of the cellular Bloch functions, and using $i\nabla_{\mathbf{k}}u_{n\mathbf{k}}(\mathbf{x}) = \sum_{n'\neq n}\mathbf{R}_{n'n}(\mathbf{k})u_{n'\mathbf{k}}(\mathbf{x})$, where $\mathbf{R}_{n'n}(\mathbf{k})$ is given in Eq. (53b), we see that $\partial I_{n_2n_1}/\partial t = \dot{\mathbf{k}}\cdot\nabla_{\mathbf{k}}I_{n_2n_1}$ promotes tunneling to states beyond n_1 and n_2. Generally, this makes the time development of $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ quite complex.

Here, in our approach, we unfold $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ of Eqs. (47a) and (47b) so as to reflect $I_{n_2n_1}$ in a relatively useful fashion. In this regard, use is made of the well-known fact [16] that $\{u_{n\mathbf{K}}\}$, for any $\mathbf{K}=\mathbf{K}_0$, span a complete set of orthonormal functions for any function periodic in the unit cell. Therefore we expand $u_{n\mathbf{K}}(\mathbf{x})$ in terms of the set $\{u_{n\mathbf{K}_0}(\mathbf{x})\}$ in the $\mathbf{K}_0$ representation [17] as

$$u_{n\mathbf{K}}(\mathbf{x}) = \sum_{n'} c_{nn'}(\mathbf{K}-\mathbf{K}_0)u_{n'\mathbf{K}_0}(\mathbf{x}), \tag{48}$$

where the coefficients $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$ are determined by the method described in Appendix A, and the $\mathbf{K}_0$ values are chosen conveniently to suit the problem at hand (usually, $\mathbf{K}_0$ is chosen to be zero thus defining the band edges). Using this representation, we can express $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ of Eq. (47a) as

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = \sum_{\mathbf{K}}\sum_{n'n''}\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)\Omega^{-1}\sum_{\mathbf{u}} c^*_{n_2n''}\left(\mathbf{k}(t)-\mathbf{K}_0-\frac{\mathbf{u}}{2}\right)c_{n_1n'}\left(\mathbf{k}(t)-\mathbf{K}_0+\frac{\mathbf{u}}{2}\right) \times\left\langle n_1,\mathbf{K}+\frac{\mathbf{u}}{2};t|\hat{f}|n_2,\mathbf{K}-\frac{\mathbf{u}}{2};t\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}}; \tag{49a}$$

here,

$$\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int_{\Omega_c} u^*_{n''\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)u_{n'\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right) \times e^{i(\mathbf{p}-\hbar\mathbf{K})\cdot\mathbf{y}/\hbar}d\mathbf{y}, \tag{49b}$$

independent of time, and $\mathbf{k}(t)$ is defined in Eq. (11b). This is exact provided we know the exact solution to the matrix equation for $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$ in Appendix A, Eq. (A8a). Using $\mathbf{u}e^{i\mathbf{u}\cdot\mathbf{x}} = -i\nabla_{\mathbf{x}}e^{i\mathbf{u}\cdot\mathbf{x}}$, we note that

$$c^*_{n_2n''}\left(\mathbf{k}(t)-\mathbf{K}_0-\frac{\mathbf{u}}{2}\right)c_{n_1n'}\left(\mathbf{k}(t)-\mathbf{K}_0+\frac{\mathbf{u}}{2}\right)e^{i\mathbf{u}\cdot\mathbf{x}} = \hat{c}^*_{n_2n''}\left(\mathbf{k}(t)-\mathbf{K}_0+\frac{i}{2}\nabla_{\mathbf{x}}\right)\hat{c}_{n_1n'}\left(\mathbf{k}(t)-\mathbf{K}_0-\frac{i}{2}\nabla_{\mathbf{x}}\right) \times e^{i\mathbf{u}\cdot\mathbf{x}}; \tag{49c}$$

then, $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ in Eq. (49a) can be expressed as

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},\mathbf{t}) = \sum_{\mathbf{K}}\hat{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{k}(t),\mathbf{K}_0,i\nabla_{\mathbf{x}})f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t), \tag{50a}$$

where

$$f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t) = \Omega^{-1}\sum_{\mathbf{u}}\left\langle n_1,\mathbf{K}+\frac{\mathbf{u}}{2};t|\hat{f}|n_2,\mathbf{K}-\frac{\mathbf{u}}{2};t\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}} \tag{50b}$$

and

$$\hat{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{k}(t),\mathbf{K}_0,i\nabla_{\mathbf{x}}) = \sum_{n'n''}\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)\hat{c}^*_{n_2n''}\left(\mathbf{k}(t)-\mathbf{K}_0+\frac{i}{2}\nabla_{\mathbf{x}}\right) \times\hat{c}_{n_1n'}\left(\mathbf{k}(t)-\mathbf{K}_0-\frac{i}{2}\nabla_{\mathbf{x}}\right). \tag{50c}$$

We see that $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ of Eqs. (50a) and (50b) exhibits a comparable form to the plane-wave based $f(\mathbf{x},\mathbf{p},t)$ of Eqs. (16a) and (16b), although here, $\hat{\Gamma}_{n_1n_2}$ reflects the role of interband cellular Bloch envelope components and $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ serves as the *reduced multiband* WDF. It is seen that the exact multiband WDF is composed of a momentum superposition of $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ and the coefficient $\hat{\Gamma}_{n_1n_2}$ of Eq. (50c), where $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ is the multiband generalization of the plane-wave WDF found in Eqs. (16a) and (16b). $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ in Eq. (50a) is a key representation of the multiband components of the WDF for Bloch dynamics in the ABR representation, and shows the importance of the so-called reduced multiband

WDF, $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$. $\hat{\Gamma}_{n_1n_2}$ in Eq. (50c), which is determined from the $\mathbf{K}_0$ representation, fully accounts for the presence of $I_{n_2n_1}$ in Eq. (47a); therefore the WDF dependence on the complete electric and magnetic field will be reflected in the quantum behavior of $f^0_{n_1n_2}$ of Eq. (50b).

Finally, from the definition of $\mathcal{I}_{n''n'}$ in Eq. (49b), we note that in expressing $u_{n\mathbf{K}_0}(\mathbf{x}\pm\mathbf{y}/2)$ as a Taylor series in $(\pm\mathbf{y}/2)$, we can therefore express the integrand of $\mathcal{I}_{n''n'}$ as a term by term explicit function of $\mathbf{y}$ and then integrate over $d\mathbf{y}$ to obtain an infinite series of delta functions in $\delta(\mathbf{p}-\hbar\mathbf{K})$ as

$$\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)=\sum_{n=0}^{\infty}\left(\frac{i\hbar}{2}\right)^n\sum_{m=0}^{n}\frac{(-1)^{n-m}}{m!(n-m)!}\times\left[(\nabla_{\mathbf{p}}\cdot\nabla_{\mathbf{x}})^{n-m}u^*_{n''\mathbf{K}_0}(\mathbf{x})\right]\left[(\nabla_{\mathbf{p}}\cdot\nabla_{\mathbf{x}})^{m}\times u_{n'\mathbf{K}_0}(\mathbf{x})\right]\delta(\mathbf{p}-\hbar\mathbf{K}).$$

This becomes

$$\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)=\mathcal{I}^{(0)}_{n''n'}(\mathbf{x},\mathbf{K}_0)\delta(\mathbf{p}-\hbar\mathbf{K})+\mathbf{I}^{(1)}_{n''n'}(\mathbf{x},\mathbf{K}_0)\cdot\nabla_{\mathbf{K}}\delta(\mathbf{p}-\hbar\mathbf{K})+\dots,\tag{50d}$$

where

$$\mathcal{I}^{(0)}_{n''n'}(\mathbf{x},\mathbf{K}_0)=u^*_{n''\mathbf{K}_0}(\mathbf{x})u_{n'\mathbf{K}_0}(\mathbf{x}),$$

$$\mathcal{I}^{(1)}_{n''n'}(\mathbf{x},\mathbf{K}_0)=\frac{1}{2i}\left[u^*_{n''\mathbf{K}_0}(\mathbf{x})\nabla_{\mathbf{x}}u_{n'\mathbf{K}_0}(\mathbf{x})-u_{n'\mathbf{K}_0}(\mathbf{x})\nabla_{\mathbf{x}}u^*_{n''\mathbf{K}_0}(\mathbf{x})\right],$$

and so forth. Thus, using $\mathcal{I}_{n''n'}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)$ of Eq. (50d) in Eq. (50c) allows for the integral over $\mathbf{K}$ in Eq. (50a) to be evaluated directly. In Sec. IV F, $\hat{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{k}(t),\mathbf{K}_0,i\nabla_{\mathbf{x}})$ of Eq. (50c) is established explicitly to first order in $(\mathbf{K}-\mathbf{K}_0)$ [Eq. (87)] although methodology is outlined for easily extending the approximation to higher orders; all coefficients are determined at a specific choice of $\mathbf{K}_0$.

It follows from Eq. (50a) that the integration of the time derivative of $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ allows for the introduction of initial conditions so that we can write

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t)=f_{n_1n_2}(\mathbf{x},\mathbf{p},t_0)+\sum_{\mathbf{K}}\left[\hat{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{k}(t),\mathbf{K}_0,i\nabla_{\mathbf{x}})\times f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)-\hat{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0,i\nabla_{\mathbf{x}})\times f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t_0)\right].\tag{51a}$$

Thus $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$, as expressed in Eq. (51a), is the complete formal result for the multiband WDF in terms of the *reduced multiband* WDF, $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$, the operator coefficient $\hat{\Gamma}_{n_1n_2}$, and their initial conditions. Further, to transform $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ of Eq. (51a) to a gauge invariant form as was done in Secs. II and III, we make use of the transformation of variables from $\mathbf{K}$ to $\boldsymbol{k}(\mathbf{x},t)$ with $f^0(\mathbf{x},\mathbf{K},t)=F^0(\mathbf{x},\boldsymbol{k},t)$ as noted in Eqs. (17) and (18), and then make use of transformations specified in Eqs. (29a)–(29c) to find that

$$\left(\mathbf{K}+\mathbf{k}_c(t)-\mathbf{K}_0\pm\frac{i}{2}\nabla_{\mathbf{x}}\right)f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)\to\left[\boldsymbol{k}(\mathbf{x},t)-\mathbf{K}_0\pm\frac{i}{2}\nabla_{\mathbf{x}}+\frac{e}{\hbar c}\mathbf{A}_2\left(\mathbf{x}\pm\frac{i}{2}\nabla_{\boldsymbol{k}}\right)\right]\times F^0_{n_1n_2}(\mathbf{x},\boldsymbol{k},t).$$

Then, Eq. (51a) becomes

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t)=f_{n_1n_2}(\mathbf{x},\mathbf{p},t_0)+\sum_{\boldsymbol{k}}\left[\tilde{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\boldsymbol{k}(\mathbf{x},t),\mathbf{K}_0,i\nabla_{\mathbf{x}})F^0_{n_1n_2}(\mathbf{x},\boldsymbol{k},t)-\tilde{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\boldsymbol{k}(\mathbf{x},t_0),\mathbf{K}_0,i\nabla_{\mathbf{x}})F^0_{n_1n_2}(\mathbf{x},\boldsymbol{k},t_0)\right],\tag{51b}$$

where

$$\tilde{\Gamma}_{n_1n_2}(\mathbf{x},\mathbf{p};\boldsymbol{k}(\mathbf{x},t),\mathbf{K}_0,i\nabla_{\mathbf{x}})=\sum_{n'n''}\mathcal{I}_{n''n'}\left(\mathbf{x},\mathbf{p}-\frac{e}{c}\mathbf{A}-\hbar\boldsymbol{k},\mathbf{K}_0\right)\times\hat{c}^*_{n_2n''}\left(\boldsymbol{k}(\mathbf{x},t)-\mathbf{K}_0+\frac{i}{2}\nabla_{\mathbf{x}}+\frac{e}{\hbar c}\mathbf{A}_2\left(\mathbf{x}+\frac{i}{2}\nabla_{\boldsymbol{k}}\right)\right)\times\hat{c}_{n_1n'}\left(\boldsymbol{k}(\mathbf{x},t)-\mathbf{K}_0-\frac{i}{2}\nabla_{\boldsymbol{k}}+\frac{e}{\hbar c}\mathbf{A}_2\left(\mathbf{x}-\frac{i}{2}\nabla_{\boldsymbol{k}}\right)\right).\tag{51c}$$

B. The reduced Wigner distribution function to $O(\mathbf{B}^2)$

Given the fundamental role of $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ as noted in Eqs. (50a) and (50b), we now proceed by treating the matrix elements of $\hat{f}$ and $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ as the essential components in examining the WDF in Bloch electron analysis. In order to obtain the lowest order, nontrivial single-band WDF using the ABR, we assume that the fields $|\mathbf{E}|$ and $|\mathbf{B}|$ are sufficiently small so that we neglect the interband matrix elements of $f^0_{n_1n_2}$. Thus we consider the matrix elements of Eq. (4) [with $C_s\{\hat{f}\}=0$] as

$$i\hbar\langle n,\mathbf{K}_1;t|\frac{\partial\hat{f}}{\partial t}|n,\mathbf{K}_2;t\rangle=\langle n,\mathbf{K}_1;t|[\hat{H},\hat{f}]|n,\mathbf{K}_2;t\rangle,\tag{52}$$

where $\langle n,\mathbf{K};t|$ are the time-dependent ABR of Eq. (44) for the energy band n. We can show [7] that

$$i\hbar\frac{\partial}{\partial t}\psi_{n\mathbf{K}}(\mathbf{x},t)=\mathbf{F}(t)\cdot\sum_{n'\neq n}\mathbf{R}_{n'n}(\mathbf{k}(t))\psi_{n'\mathbf{K}}(\mathbf{x},t),\tag{53a}$$

with $\mathbf{F}(t)=e\mathbf{E}(t)$; here, $\mathbf{R}_{n'n}(\mathbf{K})=\mathbf{R}^*_{nn'}(\mathbf{K})$ is the usual band mixing integral,

$$\mathbf{R}_{n'n}(\mathbf{K})=\frac{i}{\Omega_c}\int_{\Omega_c}u^*_{n'\mathbf{K}}(\mathbf{x})\nabla_{\mathbf{K}}u_{n\mathbf{K}}(\mathbf{x})d\mathbf{x},\tag{53b}$$

and where the phases of $\psi_{n\mathbf{K}}$ are chosen [18] so that $\mathbf{R}_{nn}(\mathbf{k})=0$, a provision which assumes the crystal possesses an inversion symmetry. If inversion symmetry is broken, then $\mathbf{R}_{nn}(\mathbf{k})$ is nonzero and therefore needs to be retained; this gives rise to significant Berry phase effects [19] which will be considered in a future study. Generally, in using the instantaneous eigenstates of Eq. (44) to describe the solution of the time-dependent Schrödinger equation for the Hamiltonian of Eq. (43b), it is seen that $\mathbf{R}_{n'n}$ band mixing elements play a direct role in producing transitions between the $n\to n'$ bands. These transitions give rise to the phenomena of Zener tunneling and are prominent for only strong electric fields (Ref. [20] (Callaway) and Ref. [7]). For relatively weak electric fields, we consider $\mathbf{F}\cdot\mathbf{R}_{n'n}\simeq 0$ so that $(\partial\psi_{n\mathbf{K}}/\partial t)\simeq 0$, and the bands are effectively uncoupled. Thus, in the weak field, single-band limit, $\langle n,\mathbf{K}_1;t|\partial \hat{f}/\partial t|n,\mathbf{K}_2;t\rangle = \partial\langle n,\mathbf{K}_1;t|\hat{f}|n,\mathbf{K}_2;t\rangle/\partial t$ and Eq. (52) can be written as

$$i\hbar\frac{\partial}{\partial t}f_n(\mathbf{K}_1,\mathbf{K}_2;t) = \langle n,\mathbf{K}_1;t|[\hat{H},\hat{f}]|n,\mathbf{K}_2;t\rangle, \tag{54}$$

where $f_n(\mathbf{K}_1,\mathbf{K}_2,t) \equiv \langle n,\mathbf{K}_1;t|\hat{f}|n,\mathbf{K}_2;t\rangle$. Using $\hat{H}$ in Eq. (43a) along with $\langle n,\mathbf{K};t|$ from Eq. (44), the term $\langle n,\mathbf{K}_1;t|[\hat{H},\hat{f}]|n,\mathbf{K}_2;t\rangle$ becomes

$$\begin{aligned}
&\langle n,\mathbf{K}_1;t|[\hat{H},\hat{f}]|n,\mathbf{K}_2;t\rangle \\
&= \bigg\{\varepsilon_n^0\bigg(\mathbf{K}_1-\frac{e}{\hbar c}\mathbf{A}_1\bigg)-\varepsilon_n^0\bigg(\mathbf{K}_2-\frac{e}{\hbar c}\mathbf{A}_1\bigg) \\
&\quad+\frac{e}{2c}\bigg[\bigg(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}_1}\bigg)\cdot\mathbf{v}_n\bigg(\mathbf{K}_1-\frac{e}{\hbar c}\mathbf{A}_1\bigg) \\
&\quad-\bigg(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}_2}\bigg)\cdot\mathbf{v}_n\bigg(\mathbf{K}_2-\frac{e}{\hbar c}\mathbf{A}_1\bigg)\bigg]\bigg\}f_n(\mathbf{K}_1,\mathbf{K}_2,t) \\
&\quad+O(\mathbf{B}^2),
\end{aligned} \tag{55}$$

where $\mathbf{v}_n(\mathbf{k}) = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon_n^0(\mathbf{k})$ (necessary matrix elements of $[\hat{H},\hat{f}]$ can be found in Appendix C). Here, a contributing term of order $O(\mathbf{B}^2)$ would come from the Hamiltonian term $\frac{e^2}{2mc^2}\mathbf{A}_2^2$, but there are additional terms of $O(\mathbf{B}^2)$, which have been excluded because of the interband dependence of $\hat{f}$ in Eq. (54). Therefore a more rigorous approach for obtaining terms of order $O(\mathbf{B}^2)$ and higher would be to proceed by employing a unitary transformation [20] of Eq. (4), which diagonalizes the Hamiltonian (43a) to the desired order, here to $O(\mathbf{B}^2)$ in the magnetic field and to all orders in the electric field by utilizing the ABR. We note that Eq. (55) is the same result that we obtained for the effective Hamiltonian case of Eq. (36) when this equation is taken to $O(\mathbf{B})$. To $O(\mathbf{B})$, the quantum transport equation for the single-band WDF is

$$\begin{aligned}
&\frac{\partial}{\partial t}F_n(\mathbf{x},\mathbf{k},t)+\mathbf{v}_n(\mathbf{k})\cdot\nabla_{\mathbf{x}}F_n(\mathbf{x},\mathbf{k},t) \\
&\quad+\hbar^{-1}\bigg[e\mathbf{E}(t)+\frac{e}{c}(\mathbf{v}_n\times\mathbf{B})\bigg]\cdot\nabla_{\mathbf{k}}F_n(\mathbf{x},\mathbf{k},t)+O(\mathbf{B}^2) \\
&= 0.
\end{aligned} \tag{56}$$

If the Hamiltonian of Eq. (43a) were diagonal in the $|n,\mathbf{K};t\rangle$ representation, it would be trivial to calculate the matrix elements $[\hat{H},\hat{f}]_{n'\mathbf{K}'n\mathbf{K}}$ in Eq. (4), and, in this case, only the intraband matrix elements of $\hat{f}$ would enter into the problem. However, since this is not the case, we seek a unitary transformation, $e^{i\hat{U}}$, with the Hermitian operator $\hat{U} = \hat{U}^\dagger$, such that the Hamiltonian transforms as

$$\overline{\hat{H}} = e^{-i\hat{U}}\hat{H}e^{i\hat{U}}, \tag{57}$$

where $\overline{\hat{H}}$ is diagonal in the ABR to order of $O(\mathbf{B}^2)$. Then applying the same unitary transformation to Eq. (4) results in

$$\begin{aligned}
&i\hbar\frac{\partial\overline{\hat{f}}}{\partial t}+i\hbar\bigg[e^{-i\hat{U}}\bigg(\frac{\partial}{\partial t}e^{i\hat{U}}\bigg)\overline{\hat{f}}+\overline{\hat{f}}\bigg(\frac{\partial}{\partial t}e^{-i\hat{U}}\bigg)e^{i\hat{U}}\bigg]-[\overline{\hat{H}},\overline{\hat{f}}] \\
&= \overline{C_s}\{\overline{\hat{f}}\},
\end{aligned} \tag{58}$$

where $\overline{\hat{f}} = e^{-i\hat{U}}\hat{f}e^{i\hat{U}}$ and $\overline{C_s}$ is similarly defined. While operators transform by the unitary transformation defined by Eq. (57), it follows equivalently that the ABR state vectors transform as $\overline{|n,\mathbf{K};t\rangle} = e^{i\hat{U}}|n,\mathbf{K};t\rangle$. These state vectors could have been also utilized to establish the transformation of Eq. (4). An outline of the methodology for diagonalization of the Hamiltonian in Eq. (43a) and the determination of the matrix elements of the operator $\hat{U}$ to the desired order of approximation can be found in Appendix B. In the derivations, we express $\hat{H}$ of Eq. (43a) as

$$\hat{H} = \hat{H}_0+\beta\hat{V}_1+\beta^2V_2, \tag{59}$$

where β (dimensionless) refers to the order of the magnetic field associated with $\mathbf{A}_2$ (in the final results, we set $\beta = 1$); we also look for $\hat{U}$ as a perturbation expansion in magnetic field

$$\hat{U} = \beta\hat{U}_1+\beta^2\hat{U}_2+O(\beta^3). \tag{60}$$

The diagonal matrix elements of $\overline{\hat{H}}$ of Eq. (57) are represented as

$$(\overline{\hat{H}})_{n\mathbf{K}n\mathbf{K}} \equiv \varepsilon_{n\mathbf{K}}(\beta) = \varepsilon_n^0+\beta\varepsilon_{n,1}+\beta^2\varepsilon_{n,2}+O(\beta^3),$$

and we find, to $O(\beta^2)$,

$$\begin{aligned}
\varepsilon_{n\mathbf{K}}(\beta) &= \varepsilon_n^0(\mathbf{k})+\beta(V_1)_{n\mathbf{K}n\mathbf{K}}+\beta^2\bigg[(V_2)_{n\mathbf{K}n\mathbf{K}} \\
&\quad+\sum_{n'\neq n}\frac{|(V_1)_{n\mathbf{K}n'\mathbf{K}}|^2}{\varepsilon_{n\mathbf{k}}^0-\varepsilon_{n'\mathbf{k}}^0}\bigg].
\end{aligned} \tag{61a}$$

We note that in Eq. (61a), the term of $O(\beta^2)$ includes not only $(V_2)_{n\mathbf{K}n\mathbf{K}}$, which corresponds to $(e^2/2mc^2)\mathbf{A}_2^2$, but also includes an additional term that depends on states $n' \neq n$; this completes the correction to and including terms of order $\mathbf{B}^2$. In using the calculated matrix elements for $V_{1,2}$, which have been derived in Appendix C, we see that $\varepsilon_{n\mathbf{K}}(\beta = 1) \equiv \varepsilon_{n\mathbf{K}}$ of Eq. (61a) reduces to

$$\begin{aligned}
\varepsilon_{n\mathbf{K}} &= \varepsilon_n^0(\mathbf{k})+\frac{e}{2\hbar c}\frac{\partial\varepsilon_n^0(\mathbf{k})}{\partial\mathbf{k}}\bigg|_{\mathbf{k}=\mathbf{k}(t)}\cdot\bigg(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}}\bigg) \\
&\quad+\frac{1}{2}\bigg(\frac{e}{2\hbar c}\bigg)^2\sum_{l,m=1}^{3}\frac{\partial^2\varepsilon_n^0(\mathbf{k})}{\partial k_l\partial k_m}\bigg|_{\mathbf{k}=\mathbf{k}(t)}\bigg(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}}\bigg)_l \\
&\quad\times\bigg(\mathbf{B}\times\frac{1}{i}\nabla_{\mathbf{K}}\bigg)_m,
\end{aligned} \tag{61b}$$

where $\mathbf{k}(t) = \mathbf{K}-(e/\hbar c)\mathbf{A}_1(t) = \mathbf{K}+\mathbf{k}_c(t)$. The operator dependence of $\varepsilon_{n\mathbf{K}}$ arises typically in the crystal momentum representation [20].

C. The Liouville equation and unitary transformations

Having established in Appendix B the $\hat{U}_{1,2}$ that diagonalizes $\overline{\hat{H}}$ through $O(\mathbf{B}^2)$, we now focus on the specific form and character of the Liouville equation in Eq. (58) while using the ABR. We note from Eq. (58) the transformed Liouville equation of Eq. (4) can be expressed in compact form as

$$i\hbar\frac{\partial\overline{\hat{f}}}{\partial t}-[\overline{\hat{H}},\overline{\hat{f}}] = \overline{C}\{\overline{\hat{f}}\}+\overline{C_s}, \tag{62a}$$

where

$$\overline{C}\{\overline{\hat{f}}\} = -i\hbar\left[e^{-i\hat{U}}\left(\frac{\partial}{\partial t}e^{i\hat{U}}\right)\overline{\hat{f}} + \overline{\hat{f}}\left(\frac{\partial}{\partial t}e^{-i\hat{U}}\right)e^{i\hat{U}}\right], \quad (62b)$$

and $\overline{C_s}$ includes the explicit scattering from phonons [5]. The term $\overline{C}\{\overline{\hat{f}}\}$, which originates from the unitary transformation of $\partial\hat{f}/\partial t$ in Eq. (4), represents an internal pseudocollision term, which strongly influences the interband mixing effects. In this particular work, we focus heavily on the canonical kinematics, so we suppress the term $\overline{C_s}$ here and consider only ballistic transport; a thorough analysis of the general behavior of the term C_s has been given in context with phonons previously [7], and $\overline{C_s}$, including phonons and impurity scattering [10], will be considered in terms of Wigner transport in the electric and magnetic fields in a future companion paper.

For the analysis of $\overline{C}\{\overline{\hat{f}}\}$, it suffices to calculate the quantity in question to $O(\hat{U}^2)$; this insures that expansion terms up to and including $O(\mathbf{B}^2)$ are included. It has been previously established [21] that the operator terms in Eq. (62b) can be reduced to

$$e^{-i\hat{U}}\frac{\partial}{\partial t}e^{i\hat{U}} = i\left\{\frac{\partial\hat{U}}{\partial t}, G(i\hat{U})\right\},$$

$$\left(\frac{\partial}{\partial t}e^{-i\hat{U}}\right)e^{i\hat{U}} = \left(e^{-i\hat{U}}\frac{\partial}{\partial t}e^{i\hat{U}}\right)^{\dagger} = -i\left\{G(-i\hat{U}), \frac{\partial\hat{U}}{\partial t}\right\};$$

here $\{\hat{a},\hat{b}\}$ denotes anticommutation and

$$G(\pm i\hat{U}) \equiv \frac{e^{\pm i\hat{U}} - 1}{\pm i\hat{U}} = 1 + \frac{1}{2!}(\pm i\hat{U}) + \frac{1}{3!}(\pm i\hat{U})^2 + \dots . \quad (63a)$$

This allows us to express $\overline{C}\{\overline{\hat{f}}\}$ as

$$\overline{C}\{\overline{\hat{f}}\} = \hbar\left[\left\{\frac{\partial\hat{U}}{\partial t}, G(i\hat{U})\right\}\overline{\hat{f}} - \overline{\hat{f}}\left\{G(-i\hat{U}), \frac{\partial\hat{U}}{\partial t}\right\}\right]. \quad (63b)$$

Now, $\overline{C}\{\overline{\hat{f}}\}$ in Eq. (63b) is an exact expression in terms of the operator $\hat{U}$. To obtain $\overline{C}\{\overline{\hat{f}}\}$ to order $\hat{U}^2$, we use Eq. (63a) in Eq. (63b) and note that

$$\left\{\frac{\partial\hat{U}}{\partial t}, G(\pm i\hat{U})\right\} = 2\frac{\partial\hat{U}}{\partial t} \pm \frac{i}{2}\left\{\frac{\partial\hat{U}}{\partial t}, \hat{U}\right\} + O(\hat{U}^3).$$

We see that to $O(\hat{U}^2)$, $\overline{C}\{\overline{f}\}$ in Eq. (63b) reduces to

$$\overline{C}\{\overline{\hat{f}}\} = \hbar[(\hat{h}_1 + i\hat{h}_2)\overline{\hat{f}} - \overline{\hat{f}}(\hat{h}_1 - i\hat{h}_2)], \quad (64a)$$

where

$$\hat{h}_1 = 2\frac{\partial\hat{U}}{\partial t}, \quad \hat{h}_2 = \frac{1}{2}\left\{\hat{U}, \frac{\partial\hat{U}}{\partial t}\right\}, \quad (64b)$$

with $\hat{h}_1^{\dagger} = \hat{h}_1$ and $\hat{h}_2^{\dagger} = \hat{h}_2$. Thus the Liouville equation of Eq. (62a) with $\overline{C}_s = 0$ becomes, to second order in $\hat{U}$,

$$i\hbar\frac{\partial\overline{\hat{f}}}{\partial t} - [\overline{\hat{H}}, \overline{\hat{f}}] = \hat{H}'\overline{\hat{f}} - \overline{\hat{f}}(\hat{H}')^{\dagger}, \quad (65a)$$

where

$$\hat{H}' = \hbar(\hat{h}_1 + i\hat{h}_2), \quad (\hat{H}')^{\dagger} = \hbar(\hat{h}_1 - i\hat{h}_2). \quad (65b)$$

In taking the matrix elements of Eq. (65a) with the ABR, while remembering that the $|n,\mathbf{K};t\rangle$ are time dependent from Eq. (53a), and $\overline{\hat{H}}$ is diagonal in $|n,\mathbf{K};t\rangle$ to second order in $\mathbf{B}$, we obtain

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} &= (\varepsilon_{n_1\mathbf{K}_1} - \varepsilon_{n_2\mathbf{K}_2})\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} \\ &\quad + \sum_{n'\mathbf{K}'}\big(H''_{n_1\mathbf{K}_1n'\mathbf{K}'}\overline{f}_{n'\mathbf{K}'n_2\mathbf{K}_2} \\ &\quad - \overline{f}_{n_1\mathbf{K}_1n'\mathbf{K}'}\widetilde{H}''_{n'\mathbf{K}'n_2\mathbf{K}_2}\big), \end{aligned} \quad (66a)$$

where

$$\begin{aligned} H''_{n_1\mathbf{K}_1n'\mathbf{K}'} &= H'_{n_1\mathbf{K}_1n'\mathbf{K}'} - \mathbf{F}(t)\cdot\mathbf{R}_{n_1n'}(\mathbf{k}_1)\delta_{\mathbf{K}_1\mathbf{K}'}, \\ \widetilde{H}''_{n_1\mathbf{K}_1n'\mathbf{K}'} &= (H')^{\dagger}_{n_1\mathbf{K}_1n'\mathbf{K}'} - \mathbf{F}(t)\cdot\mathbf{R}_{n_1n'}(\mathbf{k}_1)\delta_{\mathbf{K}_1\mathbf{K}'}, \end{aligned} \quad (66b)$$

and $\varepsilon_{n\mathbf{K}}$ is given in Eq. (61b). Here, the effect of the additional $\mathbf{F}(t)$-dependent electric field term on the right-hand side of expressions in Eq. (66b) is due to the time dependence of the ABR and simply adds to the matrix elements of $\hat{H}'$ and $(\hat{H}')^{\dagger}$; the $\mathbf{F}(t)$-dependent terms generally promote Zener interband tunneling stimulated by the electric field $\mathbf{F}(t)$. In examining the off-diagonal second-order contributions of $\hat{H}'$ and $(\hat{H}')^{\dagger}$ to the total transition matrices, we will show that these terms contribute a magnetic component of $O(\mathbf{B}^2)$ to the interband tunneling.

Now, it is clear that Eq. (66a) describes all possible matrix elements of $\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$ correct to order $\hat{U}^2$. In an effort to reduce Eq. (66a) to a more tractable form, one which retains essential information, we proceed in the spirit of the Wigner-Weisskopf approximation (WWA) by retaining from the term $\sum_{n'\mathbf{K}'}(\dots)$ on the right-hand side of Eq. (66a) the terms corresponding to $n_1\mathbf{K}_1, n_2\mathbf{K}_2$, while ignoring all others; this will result in an approximate expression for the diagonal and off-diagonal matrix elements of $\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$. So, for the sum $\sum_{n'\mathbf{K}'}(\dots)$ in Eq. (66a), we get

$$\begin{aligned} \sum_{n'\mathbf{K}'}(\dots) &= H''_{n_1\mathbf{K}_1n_1\mathbf{K}_1}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} - \overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}\widetilde{H}''_{n_2\mathbf{K}_2n_2\mathbf{K}_2} \\ &\quad + H''_{n_1\mathbf{K}_1n_2\mathbf{K}_2}\overline{f}_{n_2\mathbf{K}_2n_2\mathbf{K}_2} - \overline{f}_{n_1\mathbf{K}_1n_1\mathbf{K}_1}\widetilde{H}''_{n_1\mathbf{K}_1n_2\mathbf{K}_2} \\ &\quad + \sum_{n'\mathbf{K}'\neq n_1\mathbf{K}_1,n_2\mathbf{K}_2}(\dots). \end{aligned} \quad (67)$$

Dropping the sum on the right-hand side of Eq. (67), and inserting the remainder into Eq. (66a), we get, for $n_1\mathbf{K}_1 \neq n_2\mathbf{K}_2$,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} &= (\varepsilon_{n_1\mathbf{K}_1} - \varepsilon_{n_2\mathbf{K}_2})\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} \\ &\quad + \hbar\big[(h_1 + ih_2)_{n_1\mathbf{K}_1n_1\mathbf{K}_1}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2} \\ &\quad - \overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(h_1 - ih_2)_{n_2\mathbf{K}_2n_2\mathbf{K}_2}\big] \\ &\quad + H''_{n_1\mathbf{K}_1n_2\mathbf{K}_2}\overline{f}_{n_2\mathbf{K}_2n_2\mathbf{K}_2} \\ &\quad - \overline{f}_{n_1\mathbf{K}_1n_1\mathbf{K}_1}\widetilde{H}''_{n_1\mathbf{K}_1n_2\mathbf{K}_2}; \end{aligned} \quad (68)$$

here, $\varepsilon_{n\mathbf{K}}$ is given by Eq. (61b), and the off-diagonal elements of $\hat{H}''$, $\widetilde{\hat{H}}''$ are given by Eq. (66b). Since Eq. (68) contains a mix of off-diagonal and diagonal elements of $\overline{\hat{f}}$, closure is reached for the diagonal elements of the system by setting $n_1\mathbf{K}_1 = n_2\mathbf{K}_2 = n\mathbf{K}$ in Eq. (66a) to obtain

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\overline{f}_{n_{\mathbf{K}}n\mathbf{K}} &= \hbar\big[(h_1+ih_2)_{n\mathbf{K}n\mathbf{K}}\overline{f}_{n\mathbf{K}n\mathbf{K}} - \overline{f}_{n\mathbf{K}n\mathbf{K}}(h_1-ih_2)_{n\mathbf{K}n\mathbf{K}}\big] \\ &\quad + \sum_{n'\mathbf{K}'\neq n\mathbf{K}}(H''_{n\mathbf{K}n'\mathbf{K}'}\overline{f}_{n'\mathbf{K}'n\mathbf{K}} - \overline{f}_{n\mathbf{K}n'\mathbf{K}'}\widetilde{H}''_{n'\mathbf{K}'n\mathbf{K}}); \end{aligned} \quad (69)$$

here, the diagonal term $n'\mathbf{K}' = n\mathbf{K}$ has been extracted from the term $\sum_{n'\mathbf{K}'}(\dots)$ to display the diagonal matrix elements of $\overline{\hat{f}}$ explicitly. Thus Eqs. (68) and (69) give a closed set of equations whereby, in principle, one can self-consistently solve for the approximate diagonal and off-diagonal elements of $\overline{\hat{f}}$, consistent with their respective initial conditions. Moreover, these equations contain the multiband generalization of the Liouville equation valid to $O(\hat{U}^2)$; the $\hat{U}$ dependence is expressed in the matrix elements of $\hat{H}'$ and $(\hat{H}')^\dagger$ established in Eq. (65b). The detail calculations of the matrix elements of $\hat{H}'$ and $(\hat{H}')^\dagger$ can be found in Appendix E.

D. Single-band analysis

We now consider the specific case of single-band analysis for Eqs. (68) and (69); specifically, we consider the case where $n_1 = n_2 = n$. Then, letting $\overline{f}_{n\mathbf{K}_1n\mathbf{K}_2} \equiv \overline{f}_n(\mathbf{K}_1,\mathbf{K}_2)$, Eq. (68) becomes

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2) &= (\varepsilon_{n\mathbf{K}_1}-\varepsilon_{n\mathbf{K}_2})\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2) \\ &\quad + \hbar\big[(h_1+ih_2)_{n\mathbf{K}_1n\mathbf{K}_1}\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2) \\ &\quad - (h_1-ih_2)_{n\mathbf{K}_2n\mathbf{K}_2}\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2)\big] \\ &\quad + \hbar\big[(h_1+ih_2)_{n\mathbf{K}_1n\mathbf{K}_2}\overline{f}_n(\mathbf{K}_2,\mathbf{K}_2) \\ &\quad - \overline{f}_n(\mathbf{K}_1,\mathbf{K}_1)(h_1-ih_2)_{n\mathbf{K}_1n\mathbf{K}_2}\big]. \end{aligned} \quad (70)$$

We show in Appendix E that the required diagonal matrix elements for $(\hat{h}_1 \pm i\hat{h}_2)$ in Eq. (70) are of $O(\mathbf{B}^2)$ and have dependencies only beyond n for $n' \neq n$ [see Eqs. (E3) and (E4a)]; thus, in the single-band limit, with $\mathbf{R}_{nn'} \simeq 0$, we see that

$$i\hbar\frac{\partial}{\partial t}\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2) = \big(\varepsilon_{n\mathbf{K}_1}-\varepsilon_{n\mathbf{K}_2}\big)\overline{f}_n(\mathbf{K}_1,\mathbf{K}_2), \quad (71)$$

where $\varepsilon_{n\mathbf{K}}$ is given by Eq. (61b).

In developing the WDF equation from Eq. (71), we first explicitly write down the expression for $\varepsilon_{n\mathbf{K}}$ in Eq. (61b). Then in finding the equation for $f_n^0(\mathbf{x},\mathbf{K},t)$, we proceed as in Secs. II and III; let $\mathbf{K}_1 = \mathbf{K}+\mathbf{u}/2$, $\mathbf{K}_2 = \mathbf{K}-\mathbf{u}/2$, and form

$$\begin{aligned} f_{nn}^0(\mathbf{x},\mathbf{K},t) &\equiv f_n^0(\mathbf{x},\mathbf{K},t) \\ &= \frac{1}{\Omega}\sum_{\mathbf{u}} f_n\Big(\mathbf{K}+\frac{\mathbf{u}}{2},\mathbf{K}-\frac{\mathbf{u}}{2},t\Big)e^{i\mathbf{u}\cdot\mathbf{x}}. \end{aligned} \quad (72)$$

Using Eqs. (23) and (29a)–(29c) in the same algebraic procedure as previously applied, that is, transforming from $(\mathbf{K}_1,\mathbf{K}_2)$ to $(\mathbf{K},\mathbf{u})$ variables, using

$$\frac{1}{i}\nabla_{\mathbf{u}}e^{i\mathbf{u}\cdot\mathbf{x}} = \mathbf{x}e^{i\mathbf{u}\cdot\mathbf{x}}, \quad \frac{1}{i}\nabla_{\mathbf{x}}e^{i\mathbf{u}\cdot\mathbf{x}} = \mathbf{u}e^{i\mathbf{u}\cdot\mathbf{x}},$$

integrating $f_n^0(\mathbf{x},\mathbf{K},t)$ over $\mathbf{u}$ by parts, and transforming to $\boldsymbol{k}(\mathbf{x},t) = \mathbf{K}-(e/\hbar c)\mathbf{A}(\mathbf{x},t)$ with $F_n^0(\mathbf{x},\boldsymbol{k},t) = f_n^0(\mathbf{x},\mathbf{K},t)$, we obtain the gauge invariant equation for $F_n^0(\mathbf{x},\boldsymbol{k},t)$ as

$$\begin{aligned} &\frac{\partial}{\partial t}F_n^0(\mathbf{x},\boldsymbol{k},t) + \mathbf{v}_n(\boldsymbol{k})\cdot\nabla_{\mathbf{x}}F_n^0(\mathbf{x},\boldsymbol{k},t) + \Big[e\mathbf{E}(t)+\frac{e}{c}\mathbf{v}_n(\boldsymbol{k})\times\mathbf{B}\Big] \\ &\quad \cdot\frac{1}{\hbar}\nabla_{\boldsymbol{k}}F_n^0(\mathbf{x},\boldsymbol{k},t) + O(\mathbf{B}^3) = 0. \end{aligned} \quad (73)$$

Therefore it follows that if we neglect the interband tunneling terms that arise from both the usual Zener and magnetic-induced interband tunneling, the residual Liouville equation of Eq. (71), using $\varepsilon_{n\mathbf{K}}$ of Eq. (61b) so that $\mathbf{v}_n(\mathbf{k}) = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon_{n\mathbf{K}}(\mathbf{k})$, transforms into the analogous WDF equation of Eq. (56), but valid through $O(\mathbf{B}^3)$ in the single-band, collisionless approximation. One points out here that Eq. (61b) for $\varepsilon_{n\mathbf{K}}$ is exactly what we would have obtained if we assumed an effective Hamiltonian $\hat{H} = \varepsilon[(\hat{\mathbf{p}}-(e/c)\mathbf{A})/\hbar] = \varepsilon[(\hat{\mathbf{p}}-(e/c)\mathbf{A}_1-(e/c)\mathbf{A}_2)/\hbar]$ and taken the matrix elements with respect to plane waves where $\mathbf{A}_2 = \frac{1}{2}\mathbf{B}\times\mathbf{x}$, and then expanded the result about $\mathbf{B} = 0$ to $O(\mathbf{B}^2)$, and replaced $\mathbf{x}$ by $\frac{1}{i}\nabla_{\mathbf{k}}$. It then follows that through terms to order $\mathbf{B}^2$, the interband matrix elements of $[\overline{\hat{H}},\overline{\hat{f}}]$ with respect to the ABR are diagonal in band, and are given by the same expression as one would obtain using an effective Hamiltonian given by Sec. III.

E. Multiband considerations

The multiband consideration requires the analysis of Eqs. (68) and (69), a closed set of equations for the diagonal and off-diagonal matrix elements of $\overline{\hat{f}}$ derived from the Liouville equation using the WWA. As observed in Eqs. (68) and (69), the diagonal elements of $(\hat{h}_1 \pm i\hat{h}_2)$ present in these equations give rise to terms of $O(\mathbf{B}^2)$ and a multiband dependence as determined in Appendix E. On the other hand, the off-diagonal matrix elements of $\hat{H}''$ and $\widetilde{\hat{H}}''$ present in (68) and (69) as defined by Eq. (66b) give rise to the presence of interband tunneling promoted by the electric field dependent Zener tunneling as represented by $\mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\delta_{\mathbf{K}\mathbf{K}'}$, and the magnetic component of interband tunneling that is implicitly contained in the off-diagonal matrix elements of $(\hat{h}_1 \pm i\hat{h}_2)$.

As defined in Eq. (66b), the interband terms, with $n \neq n'$, are

$$\begin{aligned} H''_{n\mathbf{K}n'\mathbf{K}'} &= \hbar(h_1+ih_2)_{n\mathbf{K}n'\mathbf{K}'} - \mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\delta_{\mathbf{K}\mathbf{K}'}, \\ \widetilde{H}''_{n\mathbf{K}n'\mathbf{K}'} &= \hbar(h_1-ih_2)_{n\mathbf{K}n'\mathbf{K}'} - \mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\delta_{\mathbf{K}\mathbf{K}'}. \end{aligned} \quad (74)$$

Using $(h_1 \pm ih_2)_{n\mathbf{K}n'\mathbf{K}'}$ from Appendix E [Eq. (E12)], we see that Eq. (74) becomes

$$\begin{aligned} H''_{n_{\mathbf{K}}n'\mathbf{K}'} &= \hbar\frac{\partial}{\partial t}\Big[2(\beta U_1+\beta^2U_2)_{n\mathbf{K}n'\mathbf{K}'} + \frac{i}{2}\beta^2\delta_{\mathbf{K}\mathbf{K}'}N_{nn'}(\mathbf{K})\Big] \\ &\quad - \mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\delta_{\mathbf{K}\mathbf{K}'}[1-2\beta^2\mathcal{G}_{nn'}(\mathbf{K})], \\ \widetilde{H}''_{n\mathbf{K}n'\mathbf{K}'} &= \hbar\frac{\partial}{\partial t}\Big[2(\beta U_1+\beta^2U_2)_{n\mathbf{K}n'\mathbf{K}'} - \frac{i}{2}\beta^2\delta_{\mathbf{K}\mathbf{K}'}N_{nn'}(\mathbf{K})\Big] \\ &\quad - \mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\delta_{\mathbf{K}\mathbf{K}'}[1-2\beta^2\mathcal{G}_{nn'}(\mathbf{K})]. \end{aligned} \quad (75)$$

As observed in Eq. (75), the first terms are time derivatives which allow for an integrating factor in Eqs. (68) and (69), and the second term has an explicit magnetic interband tunneling contribution of $O(\mathbf{B}^2)$ to the Zener tunneling term (see E. I. Blount [20]). Both $\mathcal{G}_{nn'}(\mathbf{K})$ and $N_{nn'}(\mathbf{K})$ are defined in terms of $\hat{U}$ in Eqs. (E9b) and (E11), respectively. A full treatment of the properties of Eqs. (68) and (69), including the derivation of the WDF equation, will be discussed in a companion paper; but here we present an outline of this with salient features.

The reduction of Eqs. (68) and (69), and the resulting WDF equation can be obtained to $O(\mathbf{B}^2)$ by retaining the coefficients in these equations up to $O(\mathbf{B}^2)$. To this end, making use of the commutation properties of $\hat{U}_1^2$ noted in Appendix E, we find that Eq. (68), in combination with Eq. (69), can be expressed to $O(\mathbf{B}^2)$ as

$$i\hbar\frac{\partial}{\partial t}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t) = (\varepsilon_{n_1\mathbf{K}_1} - \varepsilon_{n_2\mathbf{K}_2})\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t) + W_{n_1\mathbf{K}_1n_2\mathbf{K}_2}\overline{f}_{n_2\mathbf{K}_2}(t) - \overline{f}_{n_1\mathbf{K}_1}(t)W_{n_1\mathbf{K}_1n_2\mathbf{K}_2} - Z_{n_1\mathbf{K}_1n_2\mathbf{K}_2}\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t_0)$$
$$+ (X_{n_1\mathbf{K}_1n_2\mathbf{K}_2} - Y_{n_1\mathbf{K}_1n_2\mathbf{K}_2})\overline{f}_{n_1\mathbf{K}_1}(t_0) + (X_{n_1\mathbf{K}_1n_2\mathbf{K}_2} + Y_{n_1\mathbf{K}_1n_2\mathbf{K}_2})\overline{f}_{n_2\mathbf{K}_2}(t_0), \tag{76a}$$

with $\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t_0)$ assumed to be a constant. Here,

$$W_{n_1\mathbf{K}_1n_2\mathbf{K}_2} = 2\hbar\frac{\partial}{\partial t}U_{n_1\mathbf{K}_1n_2\mathbf{K}_2} - \mathbf{F}(t)\cdot\mathbf{R}_{n_1n_2}(\mathbf{K}_1)\delta_{\mathbf{K}_1\mathbf{K}_2}, \tag{76b}$$

with $\hat{U} = \beta\hat{U}_1 + \beta^2\hat{U}_2$, and

$$X_{n_1\mathbf{K}_1n_2\mathbf{K}_2} = \beta^2\frac{i\hbar}{2}\delta_{\mathbf{K}_1\mathbf{K}_2}\frac{\partial}{\partial t}N_{n_1n_2}(\mathbf{K}_1),$$
$$Y_{n_1\mathbf{K}_1n_2\mathbf{K}_2} = \beta^2\mathbf{F}(t)\cdot\mathbf{R}_{n_1n_2}(\mathbf{K}_1)\delta_{\mathbf{K}_1\mathbf{K}_2}\mathcal{G}_{n_1n_2}(\mathbf{K}_1),$$
$$Z_{n_1\mathbf{K}_1n_2\mathbf{K}_2} = \beta^2\frac{i\hbar}{2}\frac{\partial}{\partial t}\left[(U_1^2)_{n_1\mathbf{K}_1n_1\mathbf{K}_1} - 3(U_1^2)_{n_2\mathbf{K}_2n_2\mathbf{K}_2}\right]. \tag{76c}$$

In Eq. (76a), the following key points are noted: (1) the multiband equation for $\overline{f}_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t) \equiv \overline{f}^0_{n_1\mathbf{K}_1n_2\mathbf{K}_2}(t)$ [$\overline{f}^0$ refers to the reduced WDF of Eq. (50b)] is an inhomogeneous equation, with the inhomogeneity dependent upon $\overline{f}_{n\mathbf{K}n\mathbf{K}}(t) \equiv \overline{f}^0_{n\mathbf{K}}(t)$, the instantaneous time-dependent diagonal matrix elements, as well as the initial conditions for $\overline{f}^0_{n\mathbf{K}}(t_0)$ and $\overline{f}^0_{n\mathbf{K}n'\mathbf{K}'}(t_0)$; (2) through the definition of $W_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$ in Eq. (76b), we observe the presence of the electric Zener tunneling term,

$$\mathbf{F}(t)\cdot\mathbf{R}_{n_1n_2}(\mathbf{K}_1)\delta_{\mathbf{K}_1\mathbf{K}_2}(\overline{f}_{n_1\mathbf{K}_1}(t) - \overline{f}_{n_2\mathbf{K}_2}(t)), \tag{77a}$$

which depends on the instantaneous behavior of $\overline{f}_{n_1\mathbf{K}_1}(t)$ and $\overline{f}_{n_2\mathbf{K}_2}(t)$; as well, the lowest order contribution to magnetic breakdown is contained in the $(\partial\hat{U}_1/\partial t)$ part of $W_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$; (3) through the definition of $Y_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$ in Eq. (76c), we observe the presence of a *magnetic-induced* electric Zener tunneling term,

$$\mathbf{F}(t)\cdot\mathbf{R}_{n_1n_2}(\mathbf{K}_1)\delta_{\mathbf{K}_1\mathbf{K}_2}\mathcal{G}_{n_1n_2}(\mathbf{K}_1)(\overline{f}_{n_1\mathbf{K}_1}(t_0) - \overline{f}_{n_2\mathbf{K}_2}(t_0)), \tag{77b}$$

which depends on the initial conditions for $\overline{f}_{n_1\mathbf{K}_1}(t_0)$ and $\overline{f}_{n_2\mathbf{K}_2}(t_0)$, as well as $\mathcal{G}_{n_1n_2}(\mathbf{K}_1)$, a magnetic field-dependent variable defined in Eq. (E9b).

Lastly, in developing the reduced WDF equation for Eq. (76a), we first utilize $\varepsilon_{n\mathbf{K}}$ in Eq. (61b), with $n = (n_1,n_2)$, $\mathbf{K} = (\mathbf{K}_1,\mathbf{K}_2)$, and then let $\mathbf{K}_1 = \mathbf{K} + \mathbf{u}/2, \mathbf{K}_2 = \mathbf{K} - \mathbf{u}/2$ while using the transformations (23), and form $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ of Eq. (50b); likewise, we also transform coefficients in Eq. (76a) using

$$\omega_{n_1n_2}(\mathbf{x},\mathbf{K},t) = \Omega^{-1}\sum_{\mathbf{u}}\left\langle n_1,\mathbf{K}+\frac{\mathbf{u}}{2};t\right|W\left|n_2,\mathbf{K}-\frac{\mathbf{u}}{2};t\right\rangle e^{i\mathbf{u}\cdot\mathbf{x}}, \tag{78}$$

with inverse

$$\left\langle n_1,\mathbf{K}+\frac{\mathbf{u}}{2};t|W|n_2,\mathbf{K}-\frac{\mathbf{u}}{2};t\right\rangle = \int_\Omega d\mathbf{x}e^{-i\mathbf{u}\cdot\mathbf{x}}\omega_{n_1n_2}(\mathbf{x},\mathbf{K},t). \tag{79}$$

Thus the equation for the reduced WDF in Eq. (76a) is of the form

$$i\hbar\frac{\partial}{\partial t}\overline{f}^0_{n_1n_2}(\mathbf{x},\mathbf{K},t) = \Big\{\varepsilon^0_{n_1}(\mathbf{K}+\mathbf{k}_c) - \varepsilon^0_{n_2}(\mathbf{K}+\mathbf{k}_c) - \frac{i\hbar}{2}\Big[\big(\mathbf{v}^0_{n_1}(\mathbf{K}+\mathbf{k}_c) + \mathbf{v}^0_{n_2}(\mathbf{K}+\mathbf{k}_c)\big)\cdot\nabla_\mathbf{x}$$
$$+ \frac{e}{2c}\big(\big(\mathbf{v}^0_{n_1}(\mathbf{K}+\mathbf{k}_c) + \mathbf{v}^0_{n_2}(\mathbf{K}+\mathbf{k}_c)\big)\times\mathbf{B}\big)\cdot\nabla_\mathbf{K}\Big] - \sum_{l,m=1}^{3}\frac{\partial^2}{\partial k_l\partial k_m}\big[\varepsilon^0_{n_1}(\mathbf{K}+\mathbf{k}_c) - \varepsilon^0_{n_2}(\mathbf{K}+\mathbf{k}_c)\big]$$
$$\times\left(\nabla_\mathbf{x} + \frac{e}{2\hbar c}\mathbf{B}\times\nabla_\mathbf{K}\right)_l\left(\nabla_\mathbf{x} + \frac{e}{2\hbar c}\mathbf{B}\times\nabla_\mathbf{K}\right)_m\Big\}\overline{f}^0_{n_1n_2}(\mathbf{x},\mathbf{K},t) + \int d\mathbf{x}'\big[\omega_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K})\overline{f}^0_{n_2}(\mathbf{x}',\mathbf{K},t)$$

$$- \overline{f}^{0}_{n_1}(\mathbf{x}',\mathbf{K},t)\omega_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K})\big] - \int d\mathbf{x}' Z_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K})\overline{f}^{0}_{n_1n_2}(\mathbf{K},t_0)$$
$$+ \int d\mathbf{x}'\big\{\big[\Psi_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K}) - Y_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K})\big]\overline{f}^{0}_{n_1}(\mathbf{K},t_0)$$
$$+ \big[\Psi_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K}) + Y_{n_1n_2}(\mathbf{x}-\mathbf{x}',\mathbf{K})\big]\overline{f}^{0}_{n_2}(\mathbf{K},t_0)\big\} + O(\mathbf{B}^3). \tag{80}$$

Here, $\mathbf{v}^0_n(\mathbf{K}+\mathbf{k}_c) = \hbar^{-1}\nabla_{\mathbf{K}}\varepsilon^0_n(\mathbf{K}+\mathbf{k}_c)$, $\omega_{n_1n_2}(\mathbf{x},\mathbf{K}), \Psi_{n_1n_2}(\mathbf{x},\mathbf{K})$, $Y_{n_1n_2}(\mathbf{x},\mathbf{K})$, and $Z_{n_1n_2}(\mathbf{x},\mathbf{K})$ are the Wigner-reduced transforms of $W_{n_1\mathbf{K}_1n_2\mathbf{K}_2}, X_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$, $Y_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$, and $Z_{n_1\mathbf{K}_1n_2\mathbf{K}_2}$ as governed by the protocol for transforming from $(\mathbf{K}_1,\mathbf{K}_2)$ to $(\mathbf{K},\mathbf{u})$ along with the transform defined by Eq. (79). For the gauge invariant form of Eq. (80), we change variables from $\mathbf{K}$ to $\mathbf{k} = \mathbf{K} - (e/c)\mathbf{A}$ with $\overline{f}^{0}(\mathbf{x},\mathbf{K},t) \to \overline{F}^{0}(\mathbf{x},\mathbf{k},t)$, while using the transformation properties from Eqs. (29a)-(29c), to find

$$\left\{\frac{\partial}{\partial t} + \frac{1}{2}\big(\mathbf{v}^0_{n_1} + \mathbf{v}^0_{n_2}\big)\cdot\nabla_{\mathbf{x}} + e\left[\mathbf{E}(t) + \frac{1}{2c}\big(\mathbf{v}^0_{n_1} + \mathbf{v}^0_{n_2}\big)\times\mathbf{B}\right]\cdot\hbar^{-1}\nabla_{\boldsymbol{k}}\right\}\overline{F}^{0}_{n_1n_2}(\mathbf{x},\boldsymbol{k},t)$$
$$= \frac{1}{i\hbar}\left\{\varepsilon^0_{n_1} - \varepsilon^0_{n_2} - \sum_{l,m=1}^{3}\frac{\partial^2\big(\varepsilon^0_{n_1} - \varepsilon^0_{n_2}\big)}{\partial k_l\partial k_m}\left(\nabla_{\mathbf{x}} + \frac{e}{\hbar c}\mathbf{B}\times\nabla_{\boldsymbol{k}}\right)_l\left(\nabla_{\mathbf{x}} + \frac{e}{\hbar c}\mathbf{B}\times\nabla_{\boldsymbol{k}}\right)_m\right\}\overline{F}^{0}_{n_1n_2}(\mathbf{x},\boldsymbol{k},t)$$
$$+ \frac{1}{i\hbar}\int d\mathbf{x}'\big\{\tilde{\omega}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k})\overline{F}^{0}_{n_2}(\mathbf{x}',\boldsymbol{k},t) - \overline{F}^{0}_{n_1}(\mathbf{x}',\boldsymbol{k},t)\tilde{\omega}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k}) - \tilde{Z}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k})\overline{F}^{0}_{n_1n_2}(\boldsymbol{k}(t_0),t_0)$$
$$+ \big[\tilde{\Psi}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k}) - \tilde{Y}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k})\big]\overline{F}^{0}_{n_1}(\boldsymbol{k}(t_0),t_0) + \big[\tilde{\Psi}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k}) + \tilde{Y}_{n_1n_2}(\mathbf{x}-\mathbf{x}',\boldsymbol{k})\big]\overline{F}^{0}_{n_2}(\boldsymbol{k}(t_0),t_0)\big\} + O(\mathbf{B}^3); \tag{81}$$

here, "tilda″ indicates transformed variables $\mathbf{K} \to \boldsymbol{k} = \mathbf{K} - (e/\hbar c)\mathbf{A}$. It is noted that when $n_1 = n_2 = n$, Eq. (81) reduces to Eq. (73), the single-band equation.

F. Results for multiband WDF to first order in $(\mathbf{K} - \mathbf{K_0})$

In developing Eq. (50a) to first order in $\delta\mathbf{K} = \mathbf{K} - \mathbf{K}_0$, we note from Eq. (48) that $c_{nn'}(\mathbf{K} - \mathbf{K}_0) = (u_{n'\mathbf{K}_0}, u_{n\mathbf{K}})$, and using the $\mathbf{k}\cdot\mathbf{p}$ method for $u_{n\mathbf{K}}$ in Eq. (A9a), we determine that

$$c_{nn'}(\mathbf{K} - \mathbf{K}_0) = \delta_{nn'} + (\mathbf{K} - \mathbf{K}_0)\cdot\mathbf{L}_{n'n}(\mathbf{K}_0) + O[(\mathbf{K} - \mathbf{K}_0)^2], \tag{82}$$

where

$$\mathbf{L}_{n'n(\mathbf{K}_0)} = \frac{\hbar}{m}\frac{\mathbf{p}_{n'n}(\mathbf{K}_0)}{\varepsilon_n(\mathbf{K}_0) - \varepsilon_{n'}(\mathbf{K}_0)} = -i\mathbf{R}_{n'n}(\mathbf{K}_0). \tag{83}$$

In keeping with Eq. (49c), it follows that

$$c^*_{n_2n''}\left(\mathbf{k}(t) - \mathbf{K}_0 - \frac{\mathbf{u}}{2}\right)c_{n_1n'}\left(\mathbf{k}(t) - \mathbf{K}_0 + \frac{\mathbf{u}}{2}\right) = \delta_{n_2n''}\delta_{n_1n'} + (\mathbf{k}(t) - \mathbf{K}_0)\cdot\big[\delta_{n_2n''}\mathbf{L}_{n'n_1}(\mathbf{K}_0) + \delta_{n_1n'}\mathbf{L}^*_{n''n_2}(\mathbf{K}_0)\big]$$
$$+ \frac{1}{2}\mathbf{u}\cdot\big[\delta_{n_2n''}\mathbf{L}_{n'n_1}(\mathbf{K}_0) - \delta_{n_1n'}\mathbf{L}^*_{n''n_2}(\mathbf{K}_0)\big] + O[(\mathbf{k} - \mathbf{K}_0 \pm \mathbf{u})^2]. \tag{84}$$

Putting (84) with $\mathbf{u} \to -i\nabla_{\mathbf{x}}$ into Eq. (50a), we find

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = \sum_{\mathbf{K}}\big[I^{(0)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) + (\mathbf{k}(t) - \mathbf{K}_0)\cdot\mathbf{I}^{(1)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) - i\mathbf{I}^{(2)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)\cdot\nabla_{\mathbf{x}}\big]f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t), \tag{85}$$

where $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$ is given in Eq. (50b). $I^{(0)}_{n_1n_2}, \mathbf{I}^{(1)}_{n_1n_2}$, and $\mathbf{I}^{(2)}_{n_1n_2}$ are explicitly given by

$$I^{(0)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\,u^*_{n_2\mathbf{K}_0}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right)u_{n_1\mathbf{K}_0}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right)e^{i(\mathbf{p}-\hbar\mathbf{K})\cdot\mathbf{y}/\hbar}, \tag{86a}$$

$$\mathbf{I}^{(1)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\left[u^*_{n_2\mathbf{K}_0}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right)\mathbf{D}_{n_1\mathbf{K}_0}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) + u_{n_1\mathbf{K}_0}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right)\mathbf{D}^*_{n_2\mathbf{K}_0}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right)\right]e^{i(\mathbf{p}-\hbar\mathbf{K})\cdot\mathbf{y}/\hbar}, \tag{86b}$$

and

$$\mathbf{I}^{(2)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\left[u^*_{n_2\mathbf{K}_0}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right)\mathbf{D}_{n_1\mathbf{K}_0}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) - u_{n_1\mathbf{K}_0}\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right)\mathbf{D}^*_{n_2\mathbf{K}_0}\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right)\right]e^{i(\mathbf{p}-\hbar\mathbf{K})\cdot\mathbf{y}/\hbar}, \tag{86c}$$

where $\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})$ is given in Eq. (A9b). Thus, to first order in $\delta\mathbf{K}$, the explicit expression for $\hat{\Gamma}_{n_1n_2}$ in Eq. (50c) is

$$\hat{\Gamma}_{n_1n_2}(\mathbf{x},-i\nabla_{\mathbf{x}},\mathbf{p};\mathbf{K},\mathbf{K}_0,t) = I^{(0)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) + (\mathbf{K}-\mathbf{K}_0+\mathbf{k}_c(t))\cdot\mathbf{I}^{(1)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0) + \mathbf{I}^{(2)}_{n_1n_2}(\mathbf{x},\mathbf{p};\mathbf{K},\mathbf{K}_0)\cdot(-i\nabla_{\mathbf{x}}). \tag{87}$$

Here, we let $\mathbf{K}_0 = 0$ thereby defining the band edges. Then, the quantities $I^{(0)}_{n_1n_2}$ and $\mathbf{I}^{(i)}_{n_1n_2}$ $(i = 1,2)$ can be evaluated with

$$u_{n_{1,2}0}(\mathbf{x}) = \sum_{\mathbf{G}} A^{(n_{1,2})}_{\mathbf{G}}(0)e^{i\mathbf{G}\cdot\mathbf{x}}, \tag{88}$$

where $(u_{n_10},u_{n_20}) = \delta_{n_1,n_2}$. This completes the derivation of $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ to order $\delta\mathbf{K}$ for $\mathbf{K}_0 = 0$. Lastly, we note that to order $\delta\mathbf{K}$, we have the time evolution of $f_{n_1n_2}(\mathbf{x},\mathbf{p},t)$ as

$$\frac{\partial}{\partial t} f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = \sum_{\mathbf{K}}\left\{\mathbf{I}^{(1)}_{n_1n_2}\cdot\frac{\partial}{\partial t}\left(\mathbf{k}_c f^0_{n_1n_2}\right) + \left[I^{(0)}_{n_1n_2} + (\mathbf{K}-\mathbf{K}_0)\cdot\mathbf{I}^{(1)}_{n_1n_2} + \mathbf{I}^{(2)}_{n_1n_2}\cdot(-i\nabla_{\mathbf{x}})\right]\frac{\partial}{\partial t} f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)\right\}, \tag{89}$$

where $\mathbf{k}_c(t) = (e/\hbar)\int_0^t \mathbf{E}(t')dt'$. Integrating Eq. (89) allows us to introduce initial conditions:

$$f_{n_1n_2}(\mathbf{x},\mathbf{p},t) = f_{n_1n_2}(\mathbf{x},\mathbf{p},t_0) + \sum_{\mathbf{K}}\left\{\left[I^{(0)}_{n_1n_2} + (\mathbf{k}(t)-\mathbf{K}_0)\cdot\mathbf{I}^{(1)}_{n_1n_2} + \mathbf{I}^{(2)}_{n_1n_2}\cdot(-i\nabla_{\mathbf{x}})\right]f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)\right.$$
$$\left. - \left[I^{(0)}_{n_1n_2} + (\mathbf{K}-\mathbf{K}_0)\cdot\mathbf{I}^{(1)}_{n_1n_2} + \mathbf{I}^{(2)}_{n_1n_2}\cdot(-i\nabla_{\mathbf{x}})\right]f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t_0)\right\}, \tag{90}$$

where $\mathbf{k}(t) = \mathbf{K}+\mathbf{k}_c(t)$. Equation (90) shows explicitly that the multiband WDF depends directly upon the reduced multiband WDF, $f^0_{n_1n_2}(\mathbf{x},\mathbf{K},t)$, and its initial conditions as determined by the Liouville equation of Eq. (62a).

In the single-band case, with $n_1 = n_2 = n$ in Eq. (90), the WDF $f_{nn}(\mathbf{x},\mathbf{p},t) \equiv f_n(\mathbf{x},\mathbf{p},t)$ can be transformed from variable $\mathbf{K}$ to $\boldsymbol{k}(\mathbf{x},t)$ using the transformations of Eqs. (29a)–(29c); then the single-band reduced WDF, $F^0_n(\mathbf{x},\boldsymbol{k},t)$, will satisfy the Boltzmann-like equation of Eq. (73) to $O(\mathbf{B}^2)$. Thus, applying (29a)–(29c) and (50c) to Eq. (90) while keeping terms to $O(\mathbf{B}^2)$ only, we find

$$f_n(\mathbf{x},\mathbf{p},t) = f_n(\mathbf{x},\mathbf{p},t_0) + \sum_{\boldsymbol{k}}\left[\tilde{I}^{(0)}_{nn} + \left(\boldsymbol{k}(\mathbf{x},t)-\mathbf{K}_0\right)\cdot\tilde{\mathbf{I}}^{(1)}_{nn} + \tilde{\mathbf{I}}^{(2)}_{nn}\cdot(-i\nabla_{\mathbf{x}})\right]F^0_n(\mathbf{x},\boldsymbol{k},t)$$
$$- \left[\tilde{I}^{(0)}_{nn} + (\mathbf{K}-\mathbf{K}_0)\cdot\tilde{\mathbf{I}}^{(1)}_{nn} + \tilde{\mathbf{I}}^{(2)}_{nn}\cdot(-i\nabla_{\mathbf{x}})\right]F^0_n(\mathbf{x},\boldsymbol{k},t_0), \tag{91}$$

where

$$\tilde{I}^{(0)}_{nn}(\mathbf{x},\mathbf{p};\boldsymbol{k},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\, u^*_{n\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)u_{n\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)e^{i[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{x},t)-\hbar\boldsymbol{k}]\cdot\mathbf{y}/\hbar}, \tag{92a}$$

$$\tilde{\mathbf{I}}^{(1)}_{nn}(\mathbf{x},\mathbf{p};\boldsymbol{k},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\left[u^*_{n\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)\mathbf{D}_{n\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right) + u^*_{n\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)\mathbf{D}_{n\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)\right]e^{i[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{x},t)-\hbar\boldsymbol{k}]\cdot\mathbf{y}/\hbar}, \tag{92b}$$

and

$$\tilde{\mathbf{I}}^{(2)}_{nn}(\mathbf{x},\mathbf{p};\boldsymbol{k},\mathbf{K}_0) = (2\pi\hbar)^{-3}\int d\mathbf{y}\left[u^*_{n\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)\mathbf{D}_{n\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right) - u^*_{n\mathbf{K}_0}\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right)\mathbf{D}_{n\mathbf{K}_0}\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)\right]e^{i[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{x},t)-\hbar\boldsymbol{k}]\cdot\mathbf{y}/\hbar}. \tag{92c}$$

In Eq. (91), $F^0_n(\mathbf{x},\boldsymbol{k},t)$ is satisfied by Eq. (73). We have already noted from Eq. (A9b) that $\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})$ is expressed by Eq. (A13a). It then follows for the single-band case, when in the weak electric field limit $\mathbf{R}_{n'n}(\mathbf{K}_0) \simeq 0$, that $\tilde{\mathbf{I}}^{(1)}_{nn} = \tilde{\mathbf{I}}^{(2)}_{nn} = 0$; therefore Eq. (91) becomes, to lowest order in $\delta\mathbf{K}$,

$$f_n(\mathbf{x},\mathbf{p},t) = f_n(\mathbf{x},\mathbf{p},t_0) + \sum_{\boldsymbol{k}}\left[\tilde{I}^{(0)}_{nn}(t)F^0_n(\mathbf{x},\boldsymbol{k},t) - \tilde{I}^{(0)}_{nn}(t_0)F^0_n(\mathbf{x},\boldsymbol{k},t_0)\right], \tag{93}$$

where $\tilde{I}^{(0)}_{nn}(t)$ is given by Eq. (92a) and $F^0_n(\mathbf{x},\boldsymbol{k},t)$ is given by Eq. (73).

V. SUMMARY

Quantum transport and the associated Wigner phase space analog have been considered for Bloch electrons in homogeneous electric and magnetic fields of arbitrary time dependence. We have specifically considered the case of collisionless or ballistic transport in this work so as to focus mainly on electron kinematics and transport "streaming" to second order in the magnetic field while treating the electric field exactly. In the general formulation, starting from the Liouville equation for the density matrix, we define the first-principles WDF in terms of the instantaneous eigenstate basis and then transform to a new set of variables defined in terms of the position, kinetic momentum, and time to ensure the gauge invariance of the WDF for the uniform magnetic field.

Our methodology for constructing the WDF and the associated equation of motion is explicitly demonstrated by deriving the exact WDF equation for a free electron in homogeneous electric and magnetic fields; this result is of the same form as that obtained for the collisionless Boltzmann transport equation, except that all the consequences of the WDF approach, including the specification of WDF initial conditions and associated wave packet analysis, pertains to the quantum regime. We further extend the methodology to the case of electrons described by an effective Hamiltonian for an arbitrary energy-band function. An exact equation for the WDF is obtained, but results are reduced to second order in the magnetic field for comparative analysis with the free electron case; here, we find the same form for the WDF equation as compared to the free-electron result, except that the velocity is now defined in terms of the gradient with $\mathbf{k}$ of the energy dispersion instead of free particle velocity. Lastly, we apply the methodology to the case of Bloch electrons in the presence of the electric and magnetic field. In using the ABR as our instantaneous eigenstates, we develop a multiband WDF using the $\mathbf{K}_0$ representation outlined in Appendix A; the leading term of the $\mathbf{k}\cdot\mathbf{p}$ method provides the lowest order term of the multiband WDF, which we use to analyze the single-band and multiband picture.

We show that in order to obtain results correct to second order in the magnetic field, we have to introduce the method of unitary transformations into the analysis to diagonalize the Hamiltonian using the ABR and simultaneously transform the Liouville equation to the appropriate order to obtain results. The single-band analysis using ABR and neglecting interband effects gives rise to an energy dispersion and WDF equation correct to second order in the magnetic field; the derived energy dispersion using the ABR is exactly what one would have obtained if we assumed the effective Hamiltonian in the electric and magnetic field, and taken the matrix elements with respect to plane waves, and then expanded the results to order $\mathbf{B}^2$, and replacing $\mathbf{x}$ by $\frac{1}{i}\nabla_{\mathbf{K}}$. In multiband considerations, we examined the transition matrix elements appearing in the Liouville transport equation. It is found that, in addition to the usual electric Zener tunneling term, a magnetic interband tunneling term appears of $O(\mathbf{B}^2)$ which shows the influence of the magnetic field on interband tunneling.

The results of this paper are considered to be the first of a two-part effort. In a future companion paper, we will be extending results for the WDF in the combined electric and magnetic fields to include collisional field effects from impurities and phonons with application to valley dependent transport in low-dimensional materials. Further on, we will be considering the role of broken inversion symmetry and Berry phase corrections in this problem.

APPENDIX A: THE $\mathbf{K}_0$ REPRESENTATION [17]

The Schrödinger equation for the Bloch wave is

$$\hat{H}_0\psi_{n\mathbf{K}}(\mathbf{x}) = \varepsilon_{n\mathbf{K}}\psi_{n\mathbf{K}}(\mathbf{x}). \tag{A1}$$

Here, $\hat{H}_0$ is the one-electron Hamiltonian which is periodic in the crystal. If we exclude spin-orbit interaction, the Hamiltonian is

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + V_c(\mathbf{x}),$$

where $V_c(\mathbf{x})$ is the periodic potential of the crystal. Since $\psi_{n\mathbf{K}}(\mathbf{x}) = \Omega^{-1/2}e^{i\mathbf{K}\cdot\mathbf{x}}u_{n\mathbf{K}}(\mathbf{x})$, Eq. (A1) may be written in terms of the cell periodic function $u_{n\mathbf{K}}(\mathbf{x})$ as

$$\hat{H}(\mathbf{K})u_{n\mathbf{K}}(\mathbf{x}) = \varepsilon_{n\mathbf{K}}u_{n\mathbf{K}}(\mathbf{x}), \tag{A2}$$

where $\hat{H}(\mathbf{K}) = e^{-i\mathbf{K}\cdot\mathbf{x}}\hat{H}_0 e^{i\mathbf{K}\cdot\mathbf{x}}$, or

$$\hat{H}(\mathbf{K}) = \hat{H}_0 + \frac{\hbar}{m}\mathbf{K}\cdot\hat{\mathbf{p}} + \frac{\hbar^2\mathbf{K}^2}{2m}. \tag{A3}$$

Note that if spin-orbit interaction is included in $\hat{H}_0$, then $\hat{H}(\mathbf{K})$ is still a polynomial of second degree in the components of $\mathbf{K}$. In letting $\mathbf{K} = \mathbf{K}_0$, we see that Eq. (A2) becomes

$$\hat{H}(\mathbf{K}_0)u_{n\mathbf{K}_0}(\mathbf{x}) = \varepsilon_{n\mathbf{K}_0}u_{n\mathbf{K}_0}(\mathbf{x}), \tag{A4}$$

where

$$\hat{H}(\mathbf{K}_0) = \hat{H}_0 + \frac{\hbar}{m}\mathbf{K}_0\cdot\hat{\mathbf{p}} + \frac{\hbar^2K_0^2}{2m}. \tag{A5}$$

In solving for $\hat{H}_0$ in Eq. (A5) and eliminating it from (A3), we see that Eq. (A2) becomes

$$\left[\hat{H}(\mathbf{K}_0) + \frac{\hbar}{m}(\mathbf{K}-\mathbf{K}_0)\cdot\hat{\mathbf{p}} + \frac{\hbar^2}{2m}\left(K^2 - K_0^2\right)\right]u_{n\mathbf{K}}(\mathbf{x}) = \varepsilon_{n\mathbf{K}}u_{n\mathbf{K}}(\mathbf{x}). \tag{A6}$$

It is well known [16] that the $u_{n\mathbf{K}}(\mathbf{x})$, for any value of $\mathbf{K} = \mathbf{K}_0$, span a complete set of orthonormal functions for any function having the same periodicity of the lattice. Therefore we can express $u_{n\mathbf{K}}(\mathbf{x})$ in Eq. (A2) as

$$u_{n\mathbf{K}}(\mathbf{x}) = \sum_{n'} c_{nn'}(\mathbf{K}-\mathbf{K}_0)u_{n'\mathbf{K}_0}(\mathbf{x}), \tag{A7}$$

where $(u_{n\mathbf{K}_0}, u_{n'\mathbf{K}_0}) = \delta_{nn'}$ and $c_{nn'}(0) = \delta_{nn'}$; the functions $u_{n\mathbf{K}_0}(\mathbf{x})$ are presumed known and satisfy Eq. (A4). Putting (A7) into Eq. (A6), multiplying both sides by $u^*_{n\mathbf{K}_0}(\mathbf{x})$ and integrating over the unit cell, we obtain

$$\sum_{n'} c_{nn'}(\mathbf{K}-\mathbf{K}_0)\left\{\left[\varepsilon_{n'\mathbf{K}_0} - \varepsilon_{n\mathbf{K}} + \frac{\hbar^2}{2m}\left(\mathbf{K}^2 - \mathbf{K}_0^2\right)\right]\delta_{nn'} + \frac{\hbar}{m}(\mathbf{K}-\mathbf{K}_0)\cdot\mathbf{p}_{nn'}(\mathbf{K}_0)\right\} = 0, \tag{A8a}$$

where the subindex n' sums over all bands and

$$\mathbf{p}_{nn'}(\mathbf{K}_0) = \frac{1}{\Omega_c}\int_{\Omega_c} u^*_{n\mathbf{K}_0}(\mathbf{x})\hat{\mathbf{p}}u_{n'\mathbf{K}_0}(\mathbf{x})d\mathbf{x}. \tag{A8b}$$

Equation (A8a) is the matrix eigenvalue equation for the point $\mathbf{K}$ in $\mathbf{K}$ space in the so-called $\mathbf{K}_0$ representation [17]; although the equation for $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$ is exact for any $\mathbf{K}$, it is most amenable to the approximate solution when $\mathbf{K}$ is chosen near $\mathbf{K}_0$, for then, the off-diagonal term can be treated as a perturbation using the $\mathbf{k}\cdot\mathbf{p}$ formalism. For simplicity here, we will consider $\mathbf{K}_0$ to be an extremum point in $\mathbf{K}$ space such that $(\nabla_{\mathbf{K}}\varepsilon_{n\mathbf{K}})_{\mathbf{K}=\mathbf{K}_0} = 0$ for all bands; the specific case of $\mathbf{K}_0 = 0$ is considered in Sec. IV F.

Although the sum $\sum_{n'}(\ldots)$ in Eq. (A8a) is over all bands, and is thus an infinite sum, the equation is amenable to perturbation theory, with $\delta\mathbf{K}\cdot\mathbf{p}_{nn'}(\mathbf{K}_0)$ as a perturbation. Then, we find to first order in $\delta\mathbf{K}=\mathbf{K}-\mathbf{K}_0$ that

$$u_{n\mathbf{K}}(\mathbf{x})=u_{n\mathbf{K}_0}(\mathbf{x})+\delta\mathbf{K}\cdot\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x}), \tag{A9a}$$

where

$$\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})=\frac{\hbar}{m}\sum_{n'\neq n}\frac{\mathbf{p}_{n'n}(\mathbf{K}_0)}{\varepsilon_{n\mathbf{K}_0}-\varepsilon_{n'\mathbf{K}_0}}u_{n'\mathbf{K}_0}(\mathbf{x}) \tag{A9b}$$

and

$$\varepsilon_{n\mathbf{K}}=\varepsilon_{n\mathbf{K}_0}+\frac{\hbar}{m}\delta\mathbf{K}\cdot[\mathbf{p}_{nn}(\mathbf{K}_0)+\hbar\mathbf{K}_0]+\frac{\hbar^2}{2m}(\delta\mathbf{K})^2+\frac{\hbar^2}{m^2}\sum_{n'\neq n}\frac{[\delta\mathbf{K}\cdot\mathbf{p}_{nn'}(\mathbf{K}_0)][\delta\mathbf{K}\cdot\mathbf{p}_{n'n}(\mathbf{K}_0)]}{\varepsilon_{n\mathbf{K}_0}-\varepsilon_{n'\mathbf{K}_0}}. \tag{A10}$$

Note that the linear term vanishes since $(\psi_{n\mathbf{K}_0},\hat{\mathbf{p}}\psi_{n\mathbf{K}_0})=\mathbf{p}_{nn}(\mathbf{K}_0)+\hbar\mathbf{K}_0=m\hbar^{-1}(\nabla_{\mathbf{K}}\varepsilon_{n\mathbf{K}})_{\mathbf{K}=\mathbf{K}_0}$, which is zero since $\mathbf{K}_0$ is an extremum point in $\mathbf{K}$ space. Equations (A9a)–(A10) can be simplified. First, noting that the inverse effective-mass tensor can be expressed as

$$m_{ij}^{-1}=m^{-1}\delta_{ij}+2m^{-2}\sum_{n'\neq n}\frac{p_{nn',i}(\mathbf{K}_0)p_{n'n,j}(\mathbf{K}_0)}{\varepsilon_{n\mathbf{K}_0}-\varepsilon_{n'\mathbf{K}_0}}$$

through the f-sum rule, then Eq. (A10) takes the form

$$\varepsilon_{n\mathbf{K}}=\varepsilon_{n\mathbf{K}_0}+\frac{\hbar^2}{2}\sum_{i,j=1}^{3}\frac{\delta K_i\delta K_j}{m_{ij}}. \tag{A11}$$

Now, noting that $[\mathbf{x},\hat{H}_0]=(i\hbar/m)\hat{\mathbf{p}}$, we find that the off-diagonal matrix elements of $\mathbf{x}$ and $\hat{\mathbf{p}}$ are related by

$$(\psi_{n'\mathbf{K}_0},\mathbf{x}\psi_{n\mathbf{K}_0})=\frac{i\hbar}{m}\frac{(\psi_{n'\mathbf{K}_0},\hat{\mathbf{p}}\psi_{n\mathbf{K}_0})}{\varepsilon_{n\mathbf{K}_0}-\varepsilon_{n'\mathbf{K}_0}},\quad n'\neq n. \tag{A12a}$$

However, since, in the Bloch representation,

$$(\psi_{n'\mathbf{K}'},\mathbf{x}\psi_{n\mathbf{K}})=\left(\delta_{n'n}\frac{1}{i}\nabla_{\mathbf{K}}+\mathbf{R}_{n'n}(\mathbf{K})\right)\delta_{\mathbf{K}'\mathbf{K}},$$
$$(\psi_{n'\mathbf{K}'},\hat{\mathbf{p}}\psi_{n\mathbf{K}})=(\hbar\mathbf{K}\delta_{n'n}+\mathbf{p}_{n'n}(\mathbf{K}))\delta_{\mathbf{K}'\mathbf{K}},$$

where $\mathbf{R}_{n'n}(\mathbf{K})$ is given in Eq. (53b), it follows that Eq. (A12a) becomes

$$\mathbf{R}_{n'n}(\mathbf{K}_0)=\frac{i\hbar}{m}\frac{\mathbf{p}_{n'n}(\mathbf{K}_0)}{\varepsilon_{n\mathbf{K}_0}-\varepsilon_{n'\mathbf{K}_0}},\quad n'\neq n. \tag{A12b}$$

Thus $\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})$ in Eq. (A9b) becomes

$$\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})=-i\sum_{n'\neq n}\mathbf{R}_{n'n}(\mathbf{K}_0)u_{n'\mathbf{K}_0}(\mathbf{x}). \tag{A13a}$$

Since $\nabla_{\mathbf{K}}u_{n\mathbf{K}}(\mathbf{x})$ is a periodic function of $\mathbf{x}$, we can write

$$i\nabla_{\mathbf{K}}u_{n\mathbf{K}}(\mathbf{x})=\sum_{n'\neq n}\mathbf{R}_{n'n}(\mathbf{K})u_{n'\mathbf{K}}(\mathbf{x}); \tag{A13b}$$

[note that, in this work, the phases of $\psi_{n\mathbf{K}}(\mathbf{x})$ are chosen so that $\mathbf{R}_{nn}(\mathbf{K})=0$]. Then, $\mathbf{D}_{n\mathbf{K}_0}$ of Eq. (A13a) becomes $\mathbf{D}_{n\mathbf{K}_0}(\mathbf{x})=\nabla_{\mathbf{K}_0}u_{n\mathbf{K}_0}(\mathbf{x})$. Therefore $u_{n\mathbf{K}}(\mathbf{x})$ of Eq. (A9a) can be formally expressed as

$$u_{n\mathbf{K}}(\mathbf{x})=u_{n\mathbf{K}_0}(\mathbf{x})+(\mathbf{K}-\mathbf{K}_0)\cdot\nabla_{\mathbf{K}_0}u_{n\mathbf{K}_0}(\mathbf{x}), \tag{A13c}$$

a first-order Taylor series expansion of $u_{n\mathbf{K}}(\mathbf{x})$ about $(\mathbf{K}-\mathbf{K}_0)$; using (A13b), Eq. (A13c) can always be expressed explicitly in terms of $\mathbf{R}_{n'n}(\mathbf{K}_0)$.

In using (A12b) in Eq. (A8a), the matrix equation for $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$ can be written in a form amenable to high-order perturbation theory in $(\mathbf{K}-\mathbf{K}_0)$ as

$$\sum_{n'}c_{nn'}(\mathbf{K}-\mathbf{K}_0)\times\left\{(\varepsilon_{n'\mathbf{K}_0}-\varepsilon_{n\mathbf{K}_0})[\delta_{nn'}-i(\mathbf{K}-\mathbf{K}_0)\cdot\mathbf{R}_{nn'}(\mathbf{K}_0)]+\left[\frac{\hbar^2}{2m}(\mathbf{K}-\mathbf{K}_0)^2-(\varepsilon_{n\mathbf{K}}-\varepsilon_{n\mathbf{K}_0})\right]\delta_{nn'}\right\}=0, \tag{A14a}$$

where

$$c_{nn'}(\mathbf{K}-\mathbf{K}_0)=c_{nn'}(0)+\nabla_{\mathbf{K}}c_{nn'}(\mathbf{K}-\mathbf{K}_0)|_{\mathbf{K}=\mathbf{K}_0}\cdot(\mathbf{K}-\mathbf{K}_0)+\frac{1}{2!}\sum_{i,j=1}^{3}\left.\frac{\partial^2c_{nn'}(\mathbf{K}-\mathbf{K}_0)}{\partial K_i\partial K_j}\right|_{\mathbf{K}=\mathbf{K}_0}(K-K_0)_i\times(K-K_0)_j+O[(\mathbf{K}-\mathbf{K}_0)^3] \tag{A14b}$$

and

$$\varepsilon_{n\mathbf{K}}-\varepsilon_{n\mathbf{K}_0}=\frac{1}{2!}\sum_{i,j=1}^{3}\left.\frac{\partial^2\varepsilon_{n\mathbf{K}}}{\partial K_i\partial K_j}\right|_{\mathbf{K}=\mathbf{K}_0}(K-K_0)_i(K-K_0)_j+O[(\mathbf{K}-\mathbf{K}_0)^3], \tag{A14c}$$

with $(\nabla_{\mathbf{K}}\varepsilon_{n\mathbf{K}})_{\mathbf{K}=\mathbf{K}_0}=0$.

As an alternative to this perturbation approach, one can expand on the previous result of Eq. (A13c) and expand $u_{n\mathbf{K}}(\mathbf{x})$ in a Taylor series about $\mathbf{K}_0$ as

$$u_{n\mathbf{K}}(\mathbf{x})=\left[1+\sum_{i=1}^{3}(K-K_0)_i\frac{\partial}{\partial K_{0i}}+\frac{1}{2!}\sum_{i,j=1}^{3}(K-K_0)_i(K-K_0)_j\frac{\partial^2}{\partial K_{0i}\partial K_{0j}}\right]u_{n\mathbf{K}_0}(\mathbf{x})+O[(\mathbf{K}-\mathbf{K}_0)^3]; \tag{A15a}$$

throughout the use of $c_{nn'}(\mathbf{K}-\mathbf{K}_0)=(u_{n'\mathbf{K}_0},u_{n\mathbf{K}})$ and the repeated use of Eq. (A13b) to establish the coefficients of $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$, the Taylor series of $u_{n\mathbf{K}}$ about $(\mathbf{K}-\mathbf{K}_0)$ can be found to any desired order. Putting $u_{n\mathbf{K}}$ of Eq. (A15a) into $c_{nn'}(\mathbf{K}-\mathbf{K}_0)=(u_{n'\mathbf{K}_0},u_{n\mathbf{K}})$, we get

$$c_{nn'}(\mathbf{K}-\mathbf{K}_0)=\delta_{nn'}+(\mathbf{K}-\mathbf{K}_0)\cdot\left(u_{n'\mathbf{K}_0},\nabla_{\mathbf{K}_0}u_{n\mathbf{K}_0}\right)+\frac{1}{2!}\sum_{i,j=1}^{3}(K-K_0)_i(K-K_0)_j\times\left(u_{n'\mathbf{K}_0},\frac{\partial^2u_{n\mathbf{K}_0}}{\partial K_{0i}\partial K_{0j}}\right)+O[(\mathbf{K}-\mathbf{K}_0)^3]. \tag{A15b}$$

Using (A13b), we find

$$\left(u_{n'\mathbf{K}_0},\nabla_{\mathbf{K}_0}u_{n\mathbf{K}_0}\right) = -i\mathbf{R}_{n'n}(\mathbf{K}_0),$$
$$\left(u_{n'\mathbf{K}_0},\frac{\partial^2 u_{n\mathbf{K}_0}}{\partial K_{0l}\partial K_{0m}}\right) = -\sum_{n''} R^l_{n'n''}(\mathbf{K}_0)R^m_{n''n}(\mathbf{K}_0) - i\frac{\partial}{\partial K_{0l}}R^m_{n'n}(\mathbf{K}_0),$$

where $R^l_{n'n}(\mathbf{K}_0)$ is the lth Cartesian component of $\mathbf{R}_{n'n}(\mathbf{K}_0)$. Of course, once $c_{nn'}(\mathbf{K}-\mathbf{K}_0)$ is determined to a desired order of $(\mathbf{K}-\mathbf{K}_0)$, then $(\varepsilon_{n\mathbf{K}}-\varepsilon_{n\mathbf{K}_0})$ immediately follows from Eq. (A14a). From Eq. (A7), we use $u_{n\mathbf{k}(t)}(\mathbf{x}) = \sum_{n'} c_{nn'}(\mathbf{k}(t)-\mathbf{K}_0)u_{n'\mathbf{K}_0}(\mathbf{x})$ in Eqs. (47a) and (47b), and we find the expressions for $f_{n_1n_2}$, $f^0_{n_1n_2}$, $\hat{\Gamma}_{n_1n_2}$, and $\mathcal{I}_{n''n'}$ given in Eqs. (50a)–(50c) and (49b), respectively.

APPENDIX B: HAMILTONIAN DIAGONALIZATION BY UNITARY TRANSFORMATION

1. The general scheme

In our problem, as noted in Eq. (59), we have a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \beta\hat{V}_1 + \beta^2 V_2, \tag{B1}$$

in which the unperturbed Hamiltonian $\hat{H}_0$ is diagonal in the accelerated Bloch state representation

$$\langle n',\mathbf{K}';t|\hat{H}_0|n,\mathbf{K};t\rangle = \varepsilon^0_n(\mathbf{k}(t))\delta_{nn'}\delta_{\mathbf{K}\mathbf{K}'}. \tag{B2}$$

At the same time, the full Hamiltonian $\hat{H}$ is not diagonal in this convenient basis due to the perturbation terms of the two magnetic field potentials, V_1 and V_2. We now use the unitary transformation

$$\overline{\hat{H}} = e^{-i\hat{U}}\hat{H}e^{i\hat{U}} \tag{B3}$$

and

$$\overline{|n,\mathbf{K};t\rangle} = e^{i\hat{U}}|n,\mathbf{K};t\rangle \tag{B4}$$

to diagonalize $\hat{H}$ in Eq. (B1) to second order in $\mathbf{B}$. To this end, we expand the Hermitian operator $\hat{U}$ ($\hat{U}^\dagger = \hat{U}$) as follows:

$$\hat{U} = \beta\hat{U}_1 + \beta^2\hat{U}_2 + \cdots, \tag{B5}$$

where the subindices of $\hat{U}_i$ stand for the order of the appropriate perturbation. We thus look for $\hat{U}$ to second order in $\mathbf{B}$, which diagonalizes the Hamiltonian of Eq. (B1). Using the well-known formula

$$e^{-i\hat{U}}\hat{H}e^{i\hat{U}} = \hat{H} + i[\hat{H},\hat{U}] - \tfrac{1}{2}[[\hat{H},\hat{U}],\hat{U}] + O(\hat{U}^3), \tag{B6}$$

and putting (B1) and (B5) into Eq. (B6), we arrive at $\overline{\hat{H}}$ to $O(\mathbf{B}^2)$ as

$$\overline{\hat{H}} = \hat{H}_0 + \beta\hat{R}_1 + \beta^2\hat{R}_2, \tag{B7}$$

where

$$\hat{R}_1 = V_1 + i[\hat{H}_0,\hat{U}_1],$$
$$\hat{R}_2 = V_2 + i[\hat{H}_0,\hat{U}_2] + i[V_1,\hat{U}_1] - \tfrac{1}{2}[[\hat{H}_0,\hat{U}_1],\hat{U}_1]. \tag{B8}$$

Since $\hat{H}_0$ is already diagonal in the ABR basis, we chose $\hat{U}_i$ such that the off-diagonal matrix elements of $\hat{R}_1$ and $\hat{R}_2$ in the ABR are zero term by term. Then, from (B8) after matrix elements are taken, we see that

$$[\hat{H}_0,\hat{U}_1] = i\hat{V}_1,$$
$$[\hat{H}_0,\hat{U}_2] = iV_2 - \tfrac{1}{2}[\hat{V}_1,\hat{U}_1]. \tag{B9}$$

These equations give rise to commutator relations for $\hat{U}_i$ with $\hat{H}_0$. The right-hand side of each equation depends on the lower order terms in $\hat{U}_i$, so we thereby have a hierarchy of relations. The off-diagonal matrix elements of each operator $\hat{U}_i$ can now be found by taking the matrix elements of (B9) with respect to $\langle n,\mathbf{K};t|\ldots|n',\mathbf{K}';t\rangle$. We note that commutators of the type $[\hat{H}_0,\hat{U}_i] = \hat{A}_i$ are such that the appropriate matrix elements $\langle n,\mathbf{K};t|[\hat{H}_0,\hat{U}_i]|n',\mathbf{K}';t\rangle = \langle n,\mathbf{K};t|\hat{A}_i|n',\mathbf{K}';t\rangle$ are obtained as

$$\left(\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}'}\right)(U_i)_{n\mathbf{K}n'\mathbf{K}'} = (A_i)_{n\mathbf{K}n'\mathbf{K}'}, \tag{B10}$$

and for $n\mathbf{K} \neq n'\mathbf{K}'$

$$(U_i)_{n\mathbf{K}n'\mathbf{K}'} = \frac{(A_i)_{n\mathbf{K}n'\mathbf{K}'}}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}'}}; \tag{B11}$$

here, $\hat{A}_i$ stands for the right-hand side of equations (B9). The explicit expressions for matrix elements $(A_i)_{n\mathbf{K}n'\mathbf{K}'}$ are evaluated below.

It is clear that for $n\mathbf{K} = n'\mathbf{K}'$, the equation (B10) leaves the diagonal matrix elements $(U_i)_{n\mathbf{K}n\mathbf{K}}$ arbitrary and undecided. To determine the diagonal elements of $\hat{U}_i$ we look for the perturbed wave function for $\hat{H}$ such that $\overline{|n,\mathbf{K};t\rangle} = |n,\mathbf{K};t\rangle + |\Phi\rangle$, where the change due to the perturbation, $|\Phi\rangle$, is orthogonal to the unperturbed state, $|n,\mathbf{K};t\rangle$; then, it follows that

$$\langle n,\mathbf{K};t|\Phi\rangle = 0; \tag{B12}$$

this is frequently called intermediate normalization. Then, making use of Eq. (B4), we expand the exponent in this equation into a series, with $\hat{U}$ given in Eq. (B5), and group terms according to their order in $\mathbf{B}$, and so on. The result for $\overline{|n,\mathbf{K};t\rangle} - |n,\mathbf{K};t\rangle = |\Phi\rangle$ is

$$|\Phi\rangle = \left[\beta i\hat{U}_1 + \beta^2\left(i\hat{U}_2 - \tfrac{1}{2}\hat{U}_1^2\right)\right]|n,\mathbf{K};t\rangle. \tag{B13}$$

The diagonal matrix elements of the transformation matrix can be found from Eq. (B12) with making use of the obtained expression for $|\Phi\rangle$ (B13).

2. Off-diagonal elements of the transformation matrix

To find the explicit expressions for off-diagonal elements of the transformation matrix $U_{n\mathbf{K}n'\mathbf{K}'}$, we use Eqs. (B9) and (B11). Then, we obtain for $O(\mathbf{B})$

$$(U_1)_{n\mathbf{K}n'\mathbf{K}'} = i\frac{(V_1)_{n\mathbf{K}n'\mathbf{K}'}}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}'}} \tag{B14}$$

and for $O(\mathbf{B}^2)$

$$(U_2)_{n\mathbf{K}n'\mathbf{K}'} = \frac{i}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}'}}\Bigg[(V_2)_{n\mathbf{K}n'\mathbf{K}'} + \frac{1}{2}\sum_{n''\mathbf{K}''}{}'(V_1)_{n\mathbf{K}n''\mathbf{K}''}(V_1)_{n''\mathbf{K}''n'\mathbf{K}'} \times \left(\frac{1}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n''\mathbf{k}''}} + \frac{1}{\varepsilon^0_{n'\mathbf{k}'} - \varepsilon^0_{n''\mathbf{k}''}}\right)\Bigg], \quad \text{(B15)}$$

where "prime" in the sum means that the summation is over $(n''\mathbf{K}'') \neq (n\mathbf{K}, n'\mathbf{k}')$.

3. Diagonal elements of the transformation matrix

The diagonal elements of the transformation matrix $U_{n\mathbf{K}n\mathbf{K}}$ are evaluated from Eqs. (B12) and (B13) to the considered order in interaction with magnetic field. We reproduce them term by term in order according to Eq. (B5). So, in the lowest order in $\mathbf{B}$, we find

$$(U_1)_{n\mathbf{K}n\mathbf{K}} = 0; \quad \text{(B16)}$$

in the second order in $\mathbf{B}$, we obtain

$$(U_2)_{n\mathbf{K}n\mathbf{K}} = -\frac{i}{2}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}}. \quad \text{(B17)}$$

Clearly, it is seen that the term $(U_1)_{n\mathbf{K}n\mathbf{K}}$ is zero, whereas $(U_2)_{n\mathbf{K}n\mathbf{K}}$ depends on diagonal elements of $\hat{U}_1^2$. Then, making use of Eq. (B14), we obtain the diagonal matrix elements for $\hat{U}_2$, in the second order in $\mathbf{B}$, as

$$(U_2)_{n\mathbf{K}n\mathbf{K}} = -\frac{i}{2}\sum_{n'\mathbf{K}'\neq n\mathbf{K}}\left|\frac{(V_1)_{n\mathbf{K}n'\mathbf{K}'}}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}'}}\right|^2. \quad \text{(B18)}$$

APPENDIX C: DETERMINATION OF KEY MATRIX ELEMENTS

The required matrix elements of $\hat{U}$ are now analyzed in terms of their perturbation theory contributions defined in Eqs. (59) and (60). The particular $\hat{U}_i(\beta)$ are derived for each off-diagonal and diagonal term of perturbation [Eq. (59)] in the ABR and can be found in Appendix B, Eqs. (B14), (B15), and (B16)–(B18), respectively. For each $\hat{U}_i$, the key matrix elements depend on terms in the Hamiltonian of Eq. (43a) [see also Eq. (9)],

$$\hat{V}_1 = -\frac{e}{mc}\mathbf{A}_2\cdot\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_1\right), \quad V_2 = \frac{e^2}{2mc^2}\mathbf{A}_2^2. \quad \text{(C1)}$$

Here, $\hat{V}_1$ is the interaction of the magnetic field with the dynamic electron, and V_2 is the second order term in the magnetic field. We consider the matrix elements of $\hat{V}_1$ and V_2 in the ABR. This allows for the determination of $\hat{U}_i$ for each perturbation term.

1. Matrix elements of $\hat{V}_1(\mathbf{x},t)$

The matrix elements of $\hat{V}_1(\mathbf{x},t)$,

$$(V_1)_{n\mathbf{K}n'\mathbf{K}'} = -\frac{e}{mc}\sum_{n''\mathbf{K}''}(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}_1\right)_{n''\mathbf{K}''n'\mathbf{K}'}, \quad \text{(C2)}$$

where $\mathbf{A}_1$ and $\mathbf{A}_2$ are defined in Eqs. (7a) and (7b), respectively, are evaluated as follows:

$$\frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}_1\right)_{n''\mathbf{K}''n'\mathbf{K}'} = \mathbf{v}_{n''n'}(\mathbf{k}'(t))\delta_{\mathbf{K}''\mathbf{K}'}, \quad \text{(C3)}$$

where $\mathbf{v}_{n''n'}(\mathbf{k}')$ is well known [7], that is

$$\mathbf{v}_{n''n'}(\mathbf{k}') = \frac{1}{\hbar}\nabla_{\mathbf{k}'}\varepsilon^0_{n'\mathbf{k}'}, \quad n'' = n',$$
$$\mathbf{v}_{n''n'}(\mathbf{k}') = \frac{i}{\hbar}\left(\varepsilon^0_{n''\mathbf{k}'} - \varepsilon^0_{n'\mathbf{k}'}\right)\mathbf{R}_{n''n'}(\mathbf{k}'), \quad n'' \neq n'; \quad \text{(C4)}$$

here

$$\mathbf{R}_{n''n'}(\mathbf{k}) = \frac{i}{\Omega_c}\int_{\Omega_c} u^*_{n''\mathbf{k}}(\mathbf{x})\nabla_{\mathbf{k}}u_{n'\mathbf{k}}(\mathbf{x})d\mathbf{x} = \mathbf{R}^*_{n'n''}(\mathbf{k}). \quad \text{(C5)}$$

For $\mathbf{A}_2$ from Eq. (7b), the matrix elements are reduced to

$$(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''} = \frac{i}{2}\mathbf{B}\times\left[\nabla_{\mathbf{k}}\delta_{nn''}\delta_{\mathbf{K}\mathbf{K}''} - \frac{1}{\Omega}\int d\mathbf{x}\nabla_{\mathbf{k}}u^*_{n\mathbf{k}}(\mathbf{x})u_{n''\mathbf{k}''}(\mathbf{x})e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\mathbf{x}}\right]. \quad \text{(C6)}$$

Since

$$\frac{1}{\Omega}\int d\mathbf{x}\nabla_{\mathbf{k}}u^*_{n\mathbf{k}}(\mathbf{x})u_{n''\mathbf{k}''}(\mathbf{x})e^{-i(\mathbf{K}-\mathbf{K}'')\cdot\mathbf{x}} = \frac{\delta_{\mathbf{K}\mathbf{K}''}}{\Omega_c}\int_{\Omega_c} d\mathbf{x}\left(\nabla_{\mathbf{k}}u^*_{n\mathbf{k}}(\mathbf{x})\right)u_{n''\mathbf{k}}(\mathbf{x}), \quad \text{(C7)}$$

Eq. (C6) becomes

$$(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''} = \frac{1}{2}\mathbf{B}\times\left[i\nabla_{\mathbf{k}}\delta_{nn''} - \frac{i}{\Omega_c}\int_{\Omega_c} d\mathbf{x} \times \left(\nabla_{\mathbf{k}}u^*_{n\mathbf{k}}(\mathbf{x})\right)u_{n''\mathbf{k}}(\mathbf{x})\right]\delta_{\mathbf{K}\mathbf{K}''}. \quad \text{(C8)}$$

Taking into account that $\nabla_{\mathbf{k}}\int u^*_{n\mathbf{k}}(\mathbf{x})u_{n''\mathbf{k}}(\mathbf{x})d\mathbf{x} = 0$, we can express (C8) as

$$(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''} = \tfrac{1}{2}\mathbf{B}\times[i\nabla_{\mathbf{k}}\delta_{nn''} + \mathbf{R}_{nn''}(\mathbf{k})]\delta_{\mathbf{K}\mathbf{K}''}. \quad \text{(C9)}$$

Using (C3) and (C9) in Eq. (C2), it follows that

$$(V_1)_{n\mathbf{K}n'\mathbf{K}'} = -\frac{e}{2c}\left\{(\mathbf{B}\times i\nabla_{\mathbf{k}})\cdot\mathbf{v}_{nn'}(\mathbf{K}) + \sum_{n''\neq n}[\mathbf{B}\times\mathbf{R}_{nn''}(\mathbf{k})]\cdot\mathbf{v}_{n''n'}(\mathbf{K}')\right\}\delta_{\mathbf{K}\mathbf{K}'}. \quad \text{(C10)}$$

Noting that the second term on the right-hand side of Eq. (C10) can be written as

$$[\mathbf{B}\times\mathbf{R}_{nn''}(\mathbf{k})]\cdot\mathbf{v}_{n''n'}(\mathbf{K}') = \frac{i}{\hbar}\left(\varepsilon^0_{n''\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}}\right)[\mathbf{R}_{nn''}(\mathbf{k})\times\mathbf{R}_{n''n'}(\mathbf{k})]\cdot\mathbf{B},$$

then the sum $\sum_{n''\neq n}(\ldots)$ becomes $\sum_{n''\neq n,n'}(\ldots)$ because of the properties of $\mathbf{R}_{nn''}(\mathbf{k})$; therefore, within the WWA, we keep only terms in (n,n'), so that Eq. (C10) becomes

$$(V_1)_{n\mathbf{K}n'\mathbf{K}'} = \frac{e}{2ic}(\mathbf{B}\times\nabla_{\mathbf{K}})\cdot\mathbf{v}_{nn'}(\mathbf{K})\delta_{\mathbf{K}\mathbf{K}'}. \quad \text{(C11)}$$

2. Matrix elements of $V_2(\mathbf{x},t)$

We consider the matrix elements of $V_2(\mathbf{x},t)$,

$$(V_2)_{n\mathbf{K}n'\mathbf{K}'} = \frac{e^2}{2mc^2}\sum_{n''\mathbf{K}''}(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''}(\mathbf{A}_2)_{n''\mathbf{K}''n'\mathbf{K}'}, \quad \text{(C12)}$$

where the matrix elements $(\mathbf{A}_2)_{n\mathbf{K}n''\mathbf{K}''}$ are given in Eq. (C9). Using these matrix elements in Eq. (C12), we see that

$$\begin{aligned}(V_2)_{n\mathbf{K}n'\mathbf{K}'} = \frac{e^2}{8mc^2}\bigg\{&(\mathbf{B}\times i\nabla_{\mathbf{K}})^2\delta_{nn'}\\ &+[(\mathbf{B}\times i\nabla_{\mathbf{K}})\cdot[\mathbf{B}\times\mathbf{R}_{nn'}(\mathbf{k})]\\ &+[\mathbf{B}\times\mathbf{R}_{nn'}(\mathbf{k})]\cdot(\mathbf{B}\times i\nabla_{\mathbf{K}})]\\ &+\sum_{n''\neq n,n'}[\mathbf{B}\times\mathbf{R}_{nn''}(\mathbf{k})]\cdot[\mathbf{B}\times\mathbf{R}_{n''n'}(\mathbf{k})]\bigg\}\delta_{\mathbf{K}\mathbf{K}'}.\end{aligned} \quad \text{(C13)}$$

Dropping the terms with $n''\neq(n,n')$ in the spirit of the WWA, Eq. (C13) results in

$$\begin{aligned}(V_2)_{n\mathbf{K}n'\mathbf{K}'} &= \frac{e^2}{8mc^2}\{(\mathbf{B}\times i\nabla_{\mathbf{K}})^2\delta_{nn'}+[(\mathbf{B}\times i\nabla_{\mathbf{K}})\cdot[\mathbf{B}\times\mathbf{R}_{nn'}(\mathbf{k})]\\ &\quad+[\mathbf{B}\times\mathbf{R}_{nn'}(\mathbf{k})]\cdot(\mathbf{B}\times i\nabla_{\mathbf{K}})]\}\delta_{\mathbf{K}\mathbf{K}'}.\end{aligned} \quad \text{(C14)}$$

The matrix elements $(V_1)_{n\mathbf{K}n'\mathbf{K}'}$ and $(V_2)_{n\mathbf{K}n'\mathbf{K}'}$, reported in (C11) and (C14), retain only the contributions connecting $(n\mathbf{K},n'\mathbf{K})$ and neglect contributions for $n''\neq(n,n')$.

3. Matrix elements of the Hamiltonian

Having established all of the relevant matrix elements for our problem, we are now in a position to determine key physical quantities of the energy, $\varepsilon_{n\mathbf{K}}$. In order to express $\varepsilon_{n\mathbf{K}}(\beta)$ of Eq. (61a) in terms of the physical kinematic variables, we use the matrix elements $(V_1)_{n\mathbf{K}n'\mathbf{K}'}$ and $(V_2)_{n\mathbf{K}n'\mathbf{K}'}$, which have been evaluated in Eqs. (C11) and (C14), respectively. In particular, it follows from Eq. (C14) that

$$(V_2)_{n\mathbf{K}n\mathbf{K}} = \frac{e^2}{8mc^2}(\mathbf{B}\times i\nabla_{\mathbf{K}})^2\delta_{\mathbf{K}\mathbf{K}'}. \quad \text{(C15)}$$

Thus all terms in Eq. (61a) are straightforward to calculate except the term of the order of $\mathbf{B}^2$, which can be expressed as

$$\frac{e^2}{2mc^2}\left[(A_2)^2_{n\mathbf{K}n\mathbf{K}}-\frac{2}{m}\sum_{n'\neq n}\sum_{l=1}^{3}(A_{2l})_{n\mathbf{K}n\mathbf{K}}(p_l(\mathbf{K}))_{nn'}\times\sum_{m=1}^{3}\frac{(A_{2m})_{n\mathbf{K}n\mathbf{K}}(p_m(\mathbf{K}))_{nn'}}{\varepsilon^0_{n'\mathbf{k}}-\varepsilon^0_{n\mathbf{k}}}\right]; \quad \text{(C16)}$$

here, A_{2l} and $p_l(\mathbf{K})$ are the lth components of $\mathbf{A}_2$ and $\mathbf{p}(\mathbf{K})$. Using the f-sum rule,

$$\frac{1}{m}\sum_{n'\neq n}\frac{(p_i)_{nn'}(p_j)_{n'n}+(p_j)_{nn'}(p_i)_{n'n}}{\varepsilon^0_{n'\mathbf{k}}-\varepsilon^0_{n\mathbf{k}}} = \delta_{ij}-\frac{m}{\hbar^2}\frac{\partial^2\varepsilon^0_{n\mathbf{k}}}{\partial k_i\partial k_j}\bigg|_{\mathbf{k}=\mathbf{k}(t)}, \quad \text{(C17)}$$

we see that the expression in (C16) reduces to

$$\frac{e^2}{2\hbar^2c^2}\sum_{l,m=1}^{3}A_{2l}A_{2m}\frac{\partial^2\varepsilon^0_{n\mathbf{k}}}{\partial k_l\partial k_m}\bigg|_{\mathbf{k}=\mathbf{k}(t)}, \quad \text{(C18)}$$

where $\mathbf{A}_2=(1/2i)(\mathbf{B}\times\nabla_{\mathbf{k}})$.

APPENDIX D: EVALUATING OF $(\partial U/\partial t)_{n\mathbf{K}n'\mathbf{K}'}$

In evaluating the matrix elements in question, one must consider the time dependence of the ABR [Eq. (44)] with which the matrix elements are being taken. As such,

$$\begin{aligned}\left(\frac{\partial U}{\partial t}\right)_{n\mathbf{K}n'\mathbf{K}'} &\equiv \int d\mathbf{x}\psi^*_{n\mathbf{K}}(\mathbf{x},t)\frac{\partial\hat{U}}{\partial t}\psi_{n'\mathbf{K}'}(\mathbf{x},t)\\ &= \frac{\partial}{\partial t}\int d\mathbf{x}\psi^*_{n\mathbf{K}}(\mathbf{x},t)\hat{U}\psi_{n'\mathbf{K}'}(\mathbf{x},t)-\Delta(t),\end{aligned} \quad \text{(D1)}$$

where

$$\Delta(t) = \int d\mathbf{x}\left(\frac{\partial\psi^*_{n\mathbf{K}}}{\partial t}\hat{U}\psi_{n'\mathbf{K}'}+\psi^*_{n\mathbf{K}}\hat{U}\frac{\partial\psi_{n'\mathbf{K}'}}{\partial t}\right). \quad \text{(D2)}$$

Now, since the explicit time dependence of $\psi_{n\mathbf{K}}(\mathbf{x},t)$ gives

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\psi_{n\mathbf{K}}(\mathbf{x},t) &= \mathbf{F}(t)\cdot\mathbf{R}_{n'n}(\mathbf{k})\psi_{n'\mathbf{K}}(\mathbf{x},t)\\ &\quad+\mathbf{F}(t)\cdot\sum_{n''\neq n,n'}\mathbf{R}_{n''n}(\mathbf{k})\psi_{n''\mathbf{K}}(\mathbf{x},t),\end{aligned}$$

then $\Delta(t)$ in Eq. (D2) becomes

$$\begin{aligned}\Delta(t) = -\frac{1}{i\hbar}\int d\mathbf{x}\mathbf{F}(t)\cdot[&\mathbf{R}_{nn'}(\mathbf{k})\psi^*_{n'\mathbf{K}}\hat{U}\psi_{n'\mathbf{K}'}\\ &+\mathbf{R}_{nn'}(\mathbf{k}')\psi^*_{n\mathbf{K}}\hat{U}\psi_{n\mathbf{K}'}]+\sum_{n''\neq n,n'}(\dots).\end{aligned} \quad \text{(D3)}$$

Here, in the spirit of the WWA used throughout, we drop the sum over $n''\neq(n,n')$ and retain only term connecting (n,n'). Thus Eq. (D1) reduces to

$$\begin{aligned}\left(\frac{\partial U}{\partial t}\right)_{n\mathbf{K}n'\mathbf{K}'} &= \frac{\partial}{\partial t}(U)_{n\mathbf{K}n'\mathbf{K}'}+\frac{1}{i\hbar}\mathbf{F}(t)\\ &\quad\cdot[\mathbf{R}_{nn'}(\mathbf{k})U_{n'\mathbf{K}n'\mathbf{K}'}-\mathbf{R}_{nn'}(\mathbf{k}')U_{n\mathbf{K}n\mathbf{K}'}].\end{aligned} \quad \text{(D4)}$$

APPENDIX E: MATRIX ELEMENTS OF $(\hat{h}_1\pm i\hat{h}_2)$

In considering the matrix elements of $(\hat{h}_1\pm i\hat{h}_2)$, where $\hat{h}_1$ and $\hat{h}_2$ are given by Eq. (64b), and noting that $\hat{U}$ of Eq. (60) is expressed in orders of perturbation theory in the magnetic field parameter, β, it follows that we can express $\hat{h}_1$ and $\hat{h}_2$ in terms of $\hat{U}$ to $O(\mathbf{B}^2)$ as

$$\begin{aligned}\hat{h}_1 &= 2\left(\beta\frac{\partial\hat{U}_1}{\partial t}+\beta^2\frac{\partial\hat{U}_2}{\partial t}\right),\\ \hat{h}_2 &= \frac{\beta^2}{2}\left(\hat{U}_1\frac{\partial\hat{U}_1}{\partial t}+\frac{\partial\hat{U}_1}{\partial t}\hat{U}_1\right).\end{aligned} \quad \text{(E1)}$$

We showed in Appendix D that $(\partial U/\partial t)_{n\mathbf{K}n'\mathbf{K}'}$ can be expressed, to within the WWA, by Eq. (D4) which is used below.

In considering the diagonal matrix elements of $\hat{h}_1$ and $\hat{h}_2$ in (E1), while using Eqs. (D4), (B16), and (B17), we find

$$(h_1)_{n\mathbf{K}n\mathbf{K}} = -i\beta^2 \frac{\partial}{\partial t}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}},$$

$$(h_2)_{n\mathbf{K}n\mathbf{K}} = \frac{\beta^2}{2}\frac{\partial}{\partial t}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}}. \tag{E2}$$

Thus, from (E2), we obtain

$$(h_1 \pm i h_2)_{n\mathbf{K}n\mathbf{K}} = -i\frac{\beta^2}{2}\begin{pmatrix} a \\ b \end{pmatrix}\frac{\partial}{\partial t}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}}, \tag{E3}$$

where $a = 1$ and $b = 3$ refer to "+" and "−," respectively. Note that in (E3),

$$\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}} = \sum_{n'\mathbf{K}'}(U_1)_{n\mathbf{K}n'\mathbf{K}'}(U_1)_{n'\mathbf{K}'n\mathbf{K}} = \sum_{n'\neq n}|(U_1)_{n\mathbf{K}n'\mathbf{K}}|^2,$$

where $(U_1)_{n\mathbf{K}n'\mathbf{K}'}$ is given by Eq. (B14) in Appendix B and $(V_1)_{n\mathbf{K}n'\mathbf{K}'}$, which appears in this equation, is given by Eq. (C11) in Appendix C. Details of the calculations are found in Appendices B and C. Thus $(U_1^2)_{n\mathbf{K}n\mathbf{K}}$ can be written as

$$\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}} = \left(\frac{e}{2c}\right)^2 \sum_{n'\neq n}\left|\frac{[\mathbf{B}\times\nabla_{\mathbf{K}}]\cdot\mathbf{v}_{nn'}(\mathbf{k})}{\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}}}\right|^2, \tag{E4a}$$

where $\mathbf{v}_{nn'}(\mathbf{k})$ is defined in Eq. (C4) and depends on $\mathbf{R}_{nn'}(\mathbf{k})$, the interband coupling matrix element. Also, the time dependence of $(U_1^2)_{n\mathbf{K}n\mathbf{K}}$ in Eq. (E4a) is governed by $\mathbf{v}_{nn'}(\mathbf{k})/(\varepsilon^0_{n\mathbf{k}} - \varepsilon^0_{n'\mathbf{k}})$. Hence the diagonal matrix elements of $(\hat{h}_1 \pm i\hat{h}_2)$ depend on all states $n' \neq n$. Since $(U_1^2)_{n\mathbf{K}n\mathbf{K}}$ of Eq. (E4a) is a key operator expression in Eqs. (68) and (69), we note that $(U_1^2)_{n\mathbf{K}n\mathbf{K}}F$ [$F = F(\mathbf{x},\mathbf{K},t)$ is arbitrary] can be written as

$$\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}}F = F\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}} + \sum_{n'\neq n}\Pi_{nn'}\{F\} + O(\mathbf{B}^3), \tag{E4b}$$

where

$$\Pi_{nn'}\{F\} = \boldsymbol{\omega}_{nn'}\cdot\nabla_{\mathbf{K}}F + \alpha_{nn'}F + \boldsymbol{\gamma}^0_{nn'}\cdot\nabla_{\mathbf{K}}(\boldsymbol{\gamma}_{nn'}\cdot\nabla_{\mathbf{K}}F); \tag{E4c}$$

here,

$$\boldsymbol{\omega}_{nn'} = \left(\frac{e}{2\hbar c}\right)^2\frac{1}{g^2_{nn'}}(\mathbf{B}\times\nabla_{\mathbf{K}})\cdot\left(g_{nn'}\mathbf{R}^*_{nn'}\boldsymbol{\gamma}_{nn'} + g_{nn'}\mathbf{R}_{nn'}\boldsymbol{\gamma}^*_{nn'}\right),$$

$$\alpha_{nn'} = \left(\frac{e}{2\hbar c}\right)^2\frac{1}{g^2_{nn'}}\nabla_{\mathbf{K}}[(\mathbf{B}\times\nabla_{\mathbf{K}})\cdot(g_{nn'}\mathbf{R}_{nn'})]\cdot\boldsymbol{\gamma}^*_{nn'},$$

$$\boldsymbol{\gamma}^0_{nn'} = \left(\frac{e}{2\hbar c}\right)^2\frac{1}{g^2_{nn'}}\boldsymbol{\gamma}^*_{nn'}, \quad \boldsymbol{\gamma}_{nn'} = g_{nn'}\mathbf{R}_{nn'}\times\mathbf{B}, \tag{E5a}$$

with $g_{nn'} = \varepsilon^0_{n\mathbf{K}} - \varepsilon^0_{n'\mathbf{K}}$. From Eq. (E4b), it follows

$$\left(\frac{\partial}{\partial t}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}}\right)F = F\frac{\partial}{\partial t}\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}} + \sum_{n'\neq n}\left[\frac{\partial}{\partial t}\Pi_{nn'}\{F\} - \Pi_{nn'}\left\{\frac{\partial F}{\partial t}\right\}\right]. \tag{E5b}$$

In considering the off-diagonal matrix elements of $(\hat{h}_1 \pm i\hat{h}_2)$, we again analyze $\hat{h}_1$ and $\hat{h}_2$ of Eq. (E1) by utilizing matrix elements $(\partial U/\partial t)_{n\mathbf{K}n'\mathbf{K}'}$ of Eq. (D4) in Appendix D. First, in the evaluation of $(h_1)_{n\mathbf{K}n'\mathbf{K}'}$, we need to evaluate $(\partial U_{1,2}/\partial t)_{n\mathbf{K}n'\mathbf{K}'}$. We observe, to lowest order in the WWA, that

$$\left(\frac{\partial U_l}{\partial t}\right)_{n\mathbf{K}n'\mathbf{K}'} = \frac{\partial}{\partial t}(U_l)_{n\mathbf{K}n'\mathbf{K}'} + \frac{1}{i\hbar}\mathbf{F}(t)\cdot[\mathbf{R}_{nn'}(\mathbf{k})(U_l)_{n'\mathbf{K}n'\mathbf{K}'} - \mathbf{R}_{nn'}(\mathbf{k}')(U_l)_{n\mathbf{K}n\mathbf{K}'}], \tag{E6}$$

where $l = 1,2$. Since $(U_1)_{n\mathbf{K}n'\mathbf{K}'}$ is given in (B14) and (C11), which gives $(U_1)_{n\mathbf{K}n\mathbf{K}'} = 0$, it then follows

$$\left(\frac{\partial U_1}{\partial t}\right)_{n\mathbf{K}n'\mathbf{K}'} = \frac{\partial}{\partial t}(U_1)_{n\mathbf{K}n'\mathbf{K}'}. \tag{E7}$$

Now, from normalization condition, $(U_2)_{n\mathbf{K}n\mathbf{K}} = -(i/2)(U_1^2)_{n\mathbf{K}n\mathbf{K}}$, and

$$\left(U_1^2\right)_{n\mathbf{K}n\mathbf{K}'} = \sum_{n_1\mathbf{K}_1}(U_1)_{n\mathbf{K}n_1\mathbf{K}_1}(U_1)_{n_1\mathbf{K}_1n\mathbf{K}'} = \sum_{n_1\neq n}|(U_1)_{n\mathbf{K}n_1\mathbf{K}}|^2\delta_{\mathbf{K}\mathbf{K}'}. \tag{E8}$$

It then follows

$$\left(\frac{\partial U_2}{\partial t}\right)_{n\mathbf{K}n'\mathbf{K}'} = \frac{\partial}{\partial t}(U_2)_{n\mathbf{K}n'\mathbf{K}'} + \frac{1}{\hbar}\mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\mathcal{G}_{nn'}(\mathbf{K})\delta_{\mathbf{K}\mathbf{K}'}, \tag{E9a}$$

where

$$\mathcal{G}_{nn'}(\mathbf{K}) = \frac{1}{2}\sum_{n_1\neq n,n'}[|(U_1)_{n\mathbf{K}n_1\mathbf{K}}|^2 - |(U_1)_{n'\mathbf{K}n_1\mathbf{K}}|^2]. \tag{E9b}$$

Thus, we obtain, by making use of (E7) and (E9a),

$$(h_1)_{n\mathbf{K}n'\mathbf{K}'} = 2\left[\beta\frac{\partial}{\partial t}(\hat{U}_1)_{n\mathbf{K}n'\mathbf{K}'} + \beta^2\frac{\partial}{\partial t}(U_2)_{n\mathbf{K}n'\mathbf{K}'} + \frac{\beta^2}{\hbar}\mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\mathcal{G}_{nn'}(\mathbf{K})\delta_{\mathbf{K}\mathbf{K}'}\right] \tag{E10a}$$

and

$$(h_2)_{n\mathbf{K}n'\mathbf{K}'} = \frac{\beta^2}{2}\delta_{\mathbf{K}\mathbf{K}'}\frac{\partial}{\partial t}N_{nn'}(\mathbf{K}); \tag{E10b}$$

here,

$$N_{nn'}(\mathbf{K}) = \sum_{n_1\neq n,n'}(U_1)_{n\mathbf{K}n_1\mathbf{K}}(U_1)^*_{n'\mathbf{K}n_1\mathbf{K}}. \tag{E11}$$

It then follows from (E10a) and (E10b) that

$$(\hat{h}_1 \pm i\hat{h}_2)_{n\mathbf{K}n'\mathbf{K}'} = \frac{\partial}{\partial t}\left[2\beta(U_1)_{n\mathbf{K}n'\mathbf{K}'} + 2\beta^2(U_2)_{n\mathbf{K}n'\mathbf{K}'} \pm i\frac{\beta^2}{2}\delta_{\mathbf{K}\mathbf{K}'}N_{nn'}(\mathbf{K})\right] + \frac{2\beta^2}{\hbar}\mathbf{F}(t)\cdot\mathbf{R}_{nn'}(\mathbf{k})\mathcal{G}_{nn'}(\mathbf{K})\delta_{\mathbf{K}\mathbf{K}'}. \tag{E12}$$

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