Irreversible evolution of many-electron systems: From the quantum-Boltzmann equation toward the semi-classical Boltzmann equation

A. Gliesche and K. Maschke
Institut de Théorie des Phénomènes Physiques, École Polytechnique Fédérale, CH-1015 EPF-Lausanne, Switzerland

F. A. Reuse
Institut de Physique des Nanostructures, École Polytechnique Fédérale, CH-1015 EPF-Lausanne, Switzerland
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Starting from the quantum-Boltzmann equation derived in a previous paper, we study the irreversible evolution of an electron gas in the one-particle phase space. The connection with phase space is established by expressing one-electron states in terms of the overcomplete and nonorthogonal generating system of coherent states. By using the generalized closure relation for coherent states, as well as the fact that a one-particle operator is completely determined by the ensemble of expectation values for all coherent states, we obtain the master equations in a form that allows us to follow the evolution in phase space. This form of the master equations provides a direct link between the quantum-statistical approach and the semi-classical Boltzmann equation. The latter is obtained after a coarse-graining procedure in the one-particle phase space and by using the fact that the electron-electron interaction, as well as the interactions between the electron gas and the bath subsystems provided by phonons or photons, are local in real space.

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I. INTRODUCTION

Physical systems such as atoms, molecules, quantum dots, or solids are generally described under the assumption that their properties can be defined without referring to the rest of the world. Such a "local" approach, even though applied with apparent success, is not consistent with quantum mechanics. In fact, it is by now well known that, in contrast to a classical description, quantum mechanical states cannot be attributed to quantum subsystems (see Refs. 1–5). At first sight, this feature seems to be in conflict with our daily experience, which suggests that such a subdivision into subsystems should always be possible. For example, we generally take for granted that the physical properties of two quantum dots can be described in terms of the properties of individual dots, provided that their mutual distance is large enough. Looking through the experimental evidence, however, we see that this "classical" preconception is not really based on our knowledge of the physical properties of single systems, but that it relies, in fact, on our experience concerning the statistical evolution of ensembles of many-particle systems interacting with their statistical environment. Accordingly, the separation into subsystems like the above-mentioned quantum dots should be discussed not in terms of the properties of closed systems but rather within the framework of quantum statistics. In this context, it is worthwhile to recall that classical physics and quantum mechanics can be formulated in the same axiomatic scheme, but that classical physics is obtained by adding one more hypothesis, which leads to the separability of classical properties.[3,4] This suggests that if the classical statistical approach becomes valid in certain situations, it should be possible to derive the classical statistical description from the quantum-statistical description under some supplementary restrictions. Clearly, the understanding of these restrictions is absolutely necessary to delimit the validity regime of the classical approach. Moreover, it establishes a sound theoretical basis for the description of the transition regime between the classical and quantum behaviors. This is the basic motivation of the present work, wherein we study the dynamical decoupling of fermionic ensembles interacting with a bath to understand the connection between the quantum-statistical approach and the classical statistical approach.

In classical mechanics, the system state is described by the positions $\mathbf{q}$ and the momenta $\mathbf{p}$ of the particles constituting the system. Accordingly, the probability distribution function $f(\mathbf{p},\mathbf{q})$, which is obtained after a coarse-graining procedure in phase space,[6] determines the statistical state of a system of classical particles. Near equilibrium and under the condition that the spatial variations of these fields are sufficiently small, the evolution of $f(\mathbf{p},\mathbf{q})$ under the influence of internal and external fields is described by the classical Boltzmann equation. By adding the Pauli-exclusion principle to account for the fermionic nature of electrons, one obtains the semi-classical Boltzmann equation. The latter has been used with great success to describe, e.g., electronic transport in macroscopic solids.[7] The semi-classical description, however, breaks down for the description of mesoscopic systems such as quantum wires or quantum dots, wherein quantum effects have to be taken into account.[8,9] These effects can be treated by using the quantum transport equations based on the Green's function approach of Refs. 10 and 11. The Keldysh formalism and its applications have been extensively discussed in literature (see, e.g., Refs. 12 and 13). Presently, our aim is to establish the connection between the quantum-statistical approach and the semi-classical Boltzmann equation in a most transparent manner. For this purpose, we will use an alternative approach and start from the master equations describing the irreversible evolution of the one-particle density matrix for an N-electron system, which were derived in Ref. 14. While in Ref. 14 the evolution was derived in the basis of the eigenvectors of the one-particle Hamiltonian $H_0^{(1)}$, we will now establish the connection with the evolution in phase space by expressing the

one-particle states in terms of the overcomplete and nonorthogonal generating system of coherent states. This generating system is most convenient for our purposes since saturating the Heisenberg inequalities, the coherent states are optimally localized in phase space.[15]

The outline of the paper is as follows: In Sec. II, we resume our former results for the master equations of an N-electron system, which were presented in Ref. 14. In Sec. III, we give a list of the properties of coherent states. These properties, which are proven in Appendixes A and B, are then used to formulate the one-particle density matrix in a phase-space representation. The master equations describing the evolution of the one-particle density matrix in phase space are obtained in Sec. IV. In Sec. V, we show that an additional coarse-graining procedure in phase space leads to the semi-classical Boltzmann equation. Our final conclusions are drawn in Sec. VI.

II. MASTER EQUATION FOR THE EVOLUTION OF THE ONE-PARTICLE DENSITY MATRIX

We start from the master equations (or "quantum-Boltzmann equations") derived in Ref. 14, which describe the irreversible evolution of the coarse-grained one-particle density matrix $\bar{D}_1(t)$ of a spatially confined weakly interacting electron gas. The considered electronic subsystem A interacts with one or several bath subsystems B_j, $j=1,2,\ldots$. The interaction operators describing the electron-bath interactions may be written as

$$H_{\mathrm{int}\,j} = \sum_{\alpha} Q^{A}_{j\alpha} \otimes Q^{B_j}_{\alpha}, \tag{1}$$

where

$$Q^{A}_{j\alpha} = \sum_{\nu\nu'} c^{+}_{\nu} a^{j\nu\nu'}_{\alpha} c_{\nu'}, \tag{2}$$

$$Q^{B_j}_{\alpha} = \sum_{\mu} b^{j\mu}_{\alpha} [(d_j)^{+}_{\mu} + (d_j)_{\mu}], \tag{3}$$

and where c^{+}_{ν}, c_{ν} and $(d_j)^{+}_{\mu}, (d_j)_{\mu}$ denote the fermion and boson creation and annihilation operators, respectively. This form of the interaction operators covers most physical situations. In particular, by identifying the operators $(d_1)^{+}_{\mu}$ $((d_1)_{\mu})$ with phonon creation (annihilation) operators and the operators $(d_2)^{+}_{\mu}$ $((d_2)_{\mu})$ with photon creation (annihilation) operators, where the indices μ label the phonon or photon modes, respectively, we obtain the electron-phonon interaction Hamiltonian $H_{\mathrm{int}\,1}$ and the electron-photon interaction Hamiltonian $H_{\mathrm{int}\,2}$.

Let us denote by $\mathcal{H}$ the Hilbert space associated with the description of a single electron. The effective electron-electron interaction corresponding to a short-range screened Coulomb interaction can be written in the following form:

$$\tilde{H}_{\mathrm{int}} = \sum_{\alpha} A_{\alpha} \otimes A_{\alpha}, \quad A_{\alpha} \in \mathcal{L}(\mathcal{H}),$$

where $\mathcal{L}(\mathcal{H})$ is the vector space of linear operators acting on $\mathcal{H}$. The operators A_{α} are self-adjoint or anti-self-adjoint operators.

In the many-body formalism the operators corresponding to A_{α}, denoted by the same symbols, are represented by

$$A_{\alpha} = \sum_{\nu\mu} a^{e}_{\alpha,\nu\mu} c^{+}_{\nu} c_{\mu}.$$

In the Schrödinger picture, the quantum-Boltzmann equation derived in Ref. 14 reads as

$$\frac{d}{dt}\bar{D}_1(t) = \frac{i}{\hbar}[\bar{D}_1(t), \hat{H}^{(1)}_0(t)] + \Gamma[\bar{D}_1(t)], \tag{4}$$

where the operator $\hat{H}^{(1)}_0$ is a renormalized one-particle Hamiltonian acting on the one-particle Hilbert space $\mathcal{H}$, and where Γ is a linear superoperator acting on $\mathcal{L}(\mathcal{H})$. We thus have

$$[\Gamma(Y)]_{\nu\mu} = \sum_{\kappa\lambda} \Gamma^{\kappa\lambda}_{\nu\mu}(t) Y_{\kappa\lambda} \quad \text{with } |\nu\rangle, |\mu\rangle, |\kappa\rangle, |\lambda\rangle \in \mathcal{H}, \quad \forall \quad Y \in \mathcal{L}(\mathcal{H}), \tag{5}$$

where the vectors $|\nu\rangle, |\mu\rangle$ denote an orthonormal basis in $\mathcal{H}$.

The operator $\bar{D}_1(t)$ represents the time-averaged one-particle density matrix:

$$\hat{(\bar{D}_1)^{I}}(\bar{t}) = \frac{1}{\Delta t}\int_{t_0}^{t_0+\Delta t} dt' \hat{(D_1)^{I}}(t'), \quad \bar{t} = t_0 + \frac{\Delta t}{2}, \tag{6}$$

where the superscript $\hat{I}$ denotes the interaction picture and where the time interval Δt is chosen in such a way that the oscillations of $\hat{(D_1)^{I}}(t)$ are suppressed and only the linear contributions with respect to Δt are kept.[14,16]

In the following, we will assume that the coarse-grained one-particle density matrix $\bar{D}_1(t)$ satisfies the von Neumann conditions.[17] For the considered N-fermion system here, we have

$$\mathrm{Tr}(\bar{D}_1) = 1 \tag{7}$$

and

$$0 \leq \langle \nu | \bar{D}_1 | \nu \rangle \leq \frac{1}{N}, \quad \forall \quad |\nu\rangle \in \mathcal{H}. \tag{8}$$

Condition (8) accounts for the Pauli-exclusion principle.[17] The superoperator Γ describes the influence of the bath subsystems provided by phonons or photons on the evolution of the one-particle density matrix $\bar{D}_1$. Accounting also for the weak electron-electron interaction in metallic systems, it linearly depends on the coarse-grained one-particle density matrix $\bar{D}_1(t)$, i.e., we have[14]

$$\Gamma = \Gamma[\bar{D}_1(t)].$$

In order to avoid too clumsy expressions, this functional dependence will not be explicitly noted in the following. We will, however, sometimes note the time dependence of the superoperator Γ, which is a consequence of the functional dependence of Γ on $\bar{D}_1(t)$. In Ref. 14, the Γ superoperator has been expressed in terms of its matrix elements in the eigenbasis $|\nu\rangle \in \mathcal{H}$ of the one-particle Hamiltonian $\hat{H}^{(1)}_0$.

These basis vectors satisfy the following stationary Schrödinger equation:

$$\hat{H}_0^{(1)}|\nu\rangle = \hbar\omega_\nu|\nu\rangle.$$

Written in this basis, Eq. (4) becomes

$$\frac{d}{dt}\bar{D}_{1,\nu\mu}(t) = \frac{i}{\hbar}[\bar{D}_1(t),\hat{H}_0^{(1)}(t)]_{\nu\mu} + \sum_{\kappa\lambda}\Gamma_{\nu\mu}^{\kappa\lambda}(t)(\bar{D}_1)_{\kappa\lambda}(t). \tag{9}$$

We note that the master equations in Eq. (4) take full account of the fermionic character of the electrons. This property is guaranteed by the particular form of the coefficients $\Gamma_{\nu\mu}^{\kappa\lambda}$, which were derived in Ref. 14. For our present purposes, we need the following symmetry property:

$$\Gamma_{\nu\mu}^{\kappa\lambda} = (\Gamma_{\mu\nu}^{\lambda\kappa})^\star$$

and the following trace property:

$$\mathrm{Tr}[\Gamma(\bar{D}_1)] \equiv \sum_\nu\left(\sum_{\kappa\lambda}\Gamma_{\nu\nu}^{\kappa\lambda}(\bar{D}_1)_{\kappa\lambda}\right) = 0,$$

which guarantees conservation of the trace $\mathrm{Tr}[\bar{D}_1(t)]$ throughout the evolution of $\bar{D}_1$.

III. PHASE-SPACE DESCRIPTION OF THE ONE-PARTICLE DENSITY MATRIX $\bar{D}_1$

Equation (9) describes the coarse-grained evolution of the one-particle density matrix $\bar{D}_1$ in the basis of the eigenvectors $|\nu\rangle$ of $\hat{H}_0^{(1)}$. This description is quite different from a classical description, wherein the statistical state is described in terms of a probability distribution function $f(\mathbf{p},\mathbf{q})$ in the one-particle phase space. In order to relate the evolution of the density matrix $\bar{D}_1$ to the evolution of the electron gas in the one-particle phase space, in the following, we will abandon the basis of the eigenstates $|\nu\rangle$ of $\hat{H}_0^{(1)}$ and switch to a description in terms of coherent states, which are represented by the vectors $|\boldsymbol{\alpha}\rangle, \boldsymbol{\alpha}\in\mathbb{C}^3$. The principal properties of coherent states are resumed in Appendix A. Equation (A24) establishes a one-to-one correspondence between the parameter $\boldsymbol{\alpha}$ and the central position $\mathbf{p}$, $\mathbf{q}$ of the corresponding coherent state $|\boldsymbol{\alpha}\rangle$ in the one-particle phase space,

$$\boldsymbol{\alpha} = \frac{\Delta_q\boldsymbol{p} - i\Delta_p\boldsymbol{q}}{\hbar}. \tag{10}$$

The parameter $\Delta_q \equiv \Delta$ specifies the extension of the coherent states in the $\mathbf{q}$ directions. The corresponding extension Δ_p of the coherent state in the $\mathbf{p}$ directions is obtained from Eq. (A4),

$$\Delta_p\Delta_q = \frac{\hbar}{2}. \tag{11}$$

Thus, by saturating the Heisenberg inequalities, coherent states are optimally localized in the one-particle phase space.

The correspondence in Eq. (10) allows us to introduce the following equivalence [see Eq. (A27)]:

$$|\boldsymbol{\alpha}\rangle \equiv |\mathbf{p},\mathbf{q}\rangle. \tag{12}$$

The parameter $\Delta = \Delta_q$ will be kept constant throughout our derivations. It is therefore omitted in our above shorthand notation for the coherent states.

In the following, we will identify the coherent states by the following real parameters:

$$z \equiv \frac{1}{\sqrt{\pi}}(\mathrm{Re}(\boldsymbol{\alpha}),\ \mathrm{Im}(\boldsymbol{\alpha})), \quad z\in\mathbb{R}^6 = \left(\frac{\Delta_q}{\sqrt{\pi\hbar}}\mathbf{p}, \frac{\Delta_p}{\sqrt{\pi\hbar}}\mathbf{q}\right) \tag{13}$$

rather than by the complex vectors $\boldsymbol{\alpha}\in\mathbb{C}^3$. By also including the spin variable $s=\{\frac{1}{2},-\frac{1}{2}\}$, we thus define the following vectors:

$$|\boldsymbol{u}\rangle = |z,s\rangle \equiv |\mathbf{p}(z),\mathbf{q}(z),s\rangle, \tag{14}$$

which constitute an overcomplete generating system in the one-particle space $\mathcal{H}\otimes\mathbb{C}^2$. The arguments z in the parameters $\mathbf{p}(z)$ and $\mathbf{q}(z)$ will be omitted whenever the reference is unambiguous. From Eqs. (11), (13), and (14) we get

$$\int_{\mathcal{A}} d\boldsymbol{u}\cdots = \sum_s\int_{\mathbb{R}^6} d^6z\cdots = \sum_s\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\cdots,$$

where

$$\mathcal{A} = \{\mathbb{R}^6, s\}$$

denotes the space of integration over the $\boldsymbol{u}$ parameter including the spin variables s.

From Eq. (A38) and by accounting for the orthogonality of the spin functions, we obtain a generalized "completeness relation":

$$\int_{\mathcal{A}} d\boldsymbol{u}P(\boldsymbol{u}) = \frac{1}{(2\pi\hbar)^3}\sum_s\int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}|\mathbf{p},\mathbf{q},s\rangle\langle\mathbf{p},\mathbf{q},s| = \mathbb{1}, \tag{15}$$

where $P(\boldsymbol{u})$ denotes the projector,

$$P(\boldsymbol{u}) = |\boldsymbol{u}\rangle\langle\boldsymbol{u}|.$$

The Hilbert–Schmidt product of $P(\boldsymbol{u})$ and $P(\boldsymbol{u}')$ is given by

$$\hat{g}(\boldsymbol{u},\boldsymbol{u}') = \mathrm{Tr}[P(\boldsymbol{u})P(\boldsymbol{u}')] = |\langle\boldsymbol{u}|\boldsymbol{u}'\rangle|^2 = \hat{g}(\boldsymbol{u}',\boldsymbol{u}). \tag{16}$$

From Eq. (A36), we obtain

$$\hat{g}(\boldsymbol{u},\boldsymbol{u}') = \delta_{ss'}g(z,z'), \tag{17}$$

where

$$g(z,z') = e^{-[(\mathbf{p}-\mathbf{p}')\Delta/\hbar]^2}e^{-[(\mathbf{q}-\mathbf{q}')/2\Delta]^2}. \tag{18}$$

The function $\hat{g}(\boldsymbol{u},\boldsymbol{u}')$ satisfies the following normalization condition:

$$\int_{\mathcal{A}} d\boldsymbol{u}\hat{g}(\boldsymbol{u},\boldsymbol{u}') = \langle\boldsymbol{u}'|\boldsymbol{u}'\rangle = 1. \tag{19}$$

According to Eq. (A42), any linear one-particle operator, $X \in \mathcal{L}(\mathcal{H})$, can be expressed in the diagonal representation. This holds, in particular, for the one-particle density matrix $\bar{D}_1$, which thus can be written as

$$\bar{D}_1 = \int_{\mathcal{A}} d\boldsymbol{u}\, \rho(\boldsymbol{u}) P(\boldsymbol{u}). \tag{20}$$

From the above equation, Eq. (16), and the positivity of the one-particle density matrix (see Ref. 17), we get

$$p(\boldsymbol{u}) \equiv \mathrm{Tr}[\bar{D}_1 P(\boldsymbol{u})] = \langle \boldsymbol{u}|\bar{D}_1|\boldsymbol{u}\rangle = \int_{\mathcal{A}} d\boldsymbol{u}'\, \rho(\boldsymbol{u}') g(\boldsymbol{u},\boldsymbol{u}') \geq 0. \tag{21}$$

For a one-particle basis, $|i\rangle \in \mathcal{H}$, diagonalizing $\bar{D}_1$, we have $\langle i|\bar{D}_1|j\rangle = d_i \delta_{ij}$, where the Pauli-exclusion principle, together with Eq. (7), implies $0 \leq d_i \leq \frac{1}{N}$, and thus,

$$p(\boldsymbol{u}) = \sum_{ij} \langle \boldsymbol{u}|i\rangle\langle i|\bar{D}_1|j\rangle\langle j|\boldsymbol{u}\rangle = \sum_i d_i \langle \boldsymbol{u}|i\rangle\langle i|\boldsymbol{u}\rangle$$

$$\leq \frac{1}{N}\sum_i \langle \boldsymbol{u}|i\rangle\langle i|\boldsymbol{u}\rangle = \frac{1}{N}.$$

According to Eqs. (7) and (19), we also have

$$\mathrm{Tr}(\bar{D}_1) = \int_{\mathcal{A}} d\boldsymbol{u}\, p(\boldsymbol{u}) = \int_{\mathcal{A}} d\boldsymbol{u}\, \rho(\boldsymbol{u}) = 1. \tag{22}$$

Integral equation (21) relates the functions $p(\boldsymbol{u})$ and $\rho(\boldsymbol{u})$. In Appendix B, we discuss the properties of the solution $\rho(\boldsymbol{u})$ of this equation for given $p(\boldsymbol{u})$. We note that, in contrast to $p(\mathbf{p},\mathbf{q},s)$, the functions $\rho(\mathbf{p},\mathbf{q},s)$ are not necessarily positive everywhere in phase space.

In Sec. IV, we will express the quantum-Boltzmann equation in the generating system of coherent states.

IV. QUANTUM-BOLTZMANN EQUATION IN PHASE SPACE

In Sec. III, we have seen that the coarse-grained density matrix $\bar{D}_1$ is fully determined by the function $\rho(z,s)$, which, according to Eqs. (21), is a functional of the probabilities $p(z,s) = \langle z,s|\bar{D}_1(t)|z,s\rangle$. It is thus sufficient to determine the evolution of $p(z,s)$. From the quantum-Boltzmann equation (4), we obtain

$$\frac{d}{dt}(\langle z,s|\bar{D}_1(t)|z,s\rangle) = \langle z,s|\frac{i}{\hbar}[\bar{D}_1(t),\hat{H}_0^{(1)}(t)]|z,s\rangle + \langle z,s|\Gamma(\bar{D}_1(t))|z,s\rangle. \tag{23}$$

Equation (21) can be written as

$$p(z,s) = \langle z,s|\bar{D}_1(t)|z,s\rangle = \int_{\mathbb{R}^6} d^6z'\, \rho(z',s) g(z,z'), \tag{24}$$

where the function $g(z,z')$ is defined in Eq. (18). In Secs. IV A and IV B, we will calculate the matrix elements of the one-particle operators on the right-hand side of Eq. (23).

A. Calculation of the expectation values $\langle z,s|[\bar{D}_1(t),\hat{H}_0^{(1)}]|z,s\rangle$

The one-particle Hamiltonian $\hat{H}_0^{(1)}$ is composed of the kinetic-energy operator T and the one-particle potential V,[18]

$$\hat{H}_0 = T + V.$$

In principle, the renormalization procedure of the electron-electron interaction Hamiltonian introduces a weak time dependence of $\hat{H}_0^{(1)}$.[14] This time dependence is, however, irrelevant for the following considerations and will therefore not be explicitly noted.

For the calculation of the commutator $\langle z,s|\frac{i}{\hbar}[\bar{D}_1,\hat{H}_0^{(1)}]|z,s\rangle$, we separately treat the contributions T and V. We start with the potential part $\langle z,s|\frac{i}{\hbar}[\bar{D}_1,V]|z,s\rangle$. The operator describing the one-particle potential can be written in the following form:

$$V(\mathbf{Q}) = \int_{\mathbb{R}^3} d^3\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{Q}} \hat{V}(\mathbf{k}). \tag{25}$$

From Eq. (A30), which expresses the position operator $\mathbf{Q}$ in terms of the operators $\mathbf{A}^\dagger$ and $\mathbf{A}$, the operator relation Eq. (A21), and the commutation relations (A5), we obtain

$$e^{i\mathbf{k}\cdot\mathbf{Q}} = e^{\Delta\mathbf{k}\cdot\mathbf{A}^\dagger} e^{-\Delta\mathbf{k}\cdot\mathbf{A}} e^{-\Delta^2\mathbf{k}^2/2},$$

and with Eqs. (10), (A28), and (A36),

$$\begin{aligned}
\langle z,s|e^{i\mathbf{k}\cdot\mathbf{Q}}|z',s'\rangle &= \delta_{ss'}\langle \mathbf{p},\mathbf{q},s|e^{i\mathbf{k}\cdot\mathbf{Q}}|\mathbf{p}',\mathbf{q}',s\rangle \\
&= \delta_{ss'}\langle \mathbf{p},\mathbf{q},s|e^{\Delta\mathbf{k}\cdot\mathbf{A}^\dagger} e^{-\Delta\mathbf{k}\cdot\mathbf{A}}|\mathbf{p}',\mathbf{q}',s\rangle e^{-\Delta^2\mathbf{k}^2/2} \\
&= \delta_{ss'} e^{\Delta\mathbf{k}\cdot(\boldsymbol{\alpha}^\star - \boldsymbol{\alpha}')}\langle \mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle e^{-\Delta^2\mathbf{k}^2/2} \\
&= \delta_{ss'} e^{\Delta^2\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')/\hbar} e^{i\mathbf{k}\cdot(\mathbf{q}'+\mathbf{q})/2} \\
&\quad \times e^{-\Delta^2\mathbf{k}^2/2}\langle \mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle.
\end{aligned}$$

Accordingly, the matrix element of the potential operator Eq. (25) becomes

$$\langle \mathbf{p},\mathbf{q},s|V(\mathbf{Q})|\mathbf{p}',\mathbf{q}',s'\rangle = \delta_{ss'}\langle \mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle \int_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{V}(\mathbf{k}) \times e^{\Delta^2\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')/\hbar} e^{i\mathbf{k}\cdot(\mathbf{q}'+\mathbf{q})/2} e^{-\Delta^2\mathbf{k}^2/2}.$$

In the absence of spin-orbit coupling, the above matrix elements are independent of the spin s. Thus, for $\mathbf{q}' = \mathbf{q}$ and $\mathbf{p}' = \mathbf{p}$, the above expression reduces to

$$\langle \mathbf{p},\mathbf{q},s|V(\mathbf{Q})|\mathbf{p},\mathbf{q},s'\rangle = \delta_{ss'} \int_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{V}(\mathbf{k}) e^{-\Delta^2\mathbf{k}^2/2} e^{i\mathbf{k}\cdot\mathbf{q}}. \tag{26}$$

According to Eq. (A42), any one-particle operator is already completely determined by the above expectation values.

Thus, by taking coherent states $|\mathbf{p},\mathbf{q},s\rangle$ characterized by the parameter Δ, we can replace the original one-particle potential by the following smoothed potential:

$$V^c(\mathbf{q}) = \int_{\mathbb{R}^3} d^3\mathbf{k}\hat{V}^c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{q}}, \tag{27}$$

with the following Fourier components:

$$\hat{V}^c(\mathbf{k}) = e^{-\Delta^2\mathbf{k}^2/2}\hat{V}(\mathbf{k}).$$

By expressing $\bar{D}_1$ in the diagonal representation Eq. (20), we obtain the following for the expectation value of the commutator $[\bar{D}_1, V]$

$$\begin{aligned}
&\langle z,s|\frac{i}{\hbar}[\bar{D}_1, V(\mathbf{Q})]|z,s\rangle \\
&= \frac{i}{\hbar}(\langle z,s|\bar{D}_1 V(\mathbf{Q})|z,s\rangle - \langle z,s|V(\mathbf{Q})\bar{D}_1|z,s\rangle) \\
&= \frac{i}{\hbar}\int_{\mathbb{R}^3} d^3\mathbf{k}\hat{V}(\mathbf{k})e^{-\Delta^2\mathbf{k}^2/2}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\rho(\mathbf{p}',\mathbf{q}',s) \\
&\quad\times|\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle|^2 e^{i\mathbf{k}\cdot(\mathbf{q}+\mathbf{q}')/2} \\
&\quad\times(e^{\Delta^2\mathbf{k}\cdot(\mathbf{p}'-\mathbf{p})/\hbar} - e^{\Delta^2\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')/\hbar}).
\end{aligned} \tag{28}$$

Let us now suppose that the one-particle density matrix $\bar{D}_1(t)$ can be represented by the following functions:

$$|\rho(\boldsymbol{u})| \le M < \infty, \tag{29}$$

where M is chosen to be sufficiently small, so that

$$\begin{aligned}
&\langle\mathbf{p},\mathbf{q},s|\bar{D}_1(t)|\mathbf{p}',\mathbf{q}',s\rangle \\
&\quad\approx 0 \quad \text{for } |\mathbf{p}'-\mathbf{p}| > \Delta_p,\ |\mathbf{q}'-\mathbf{q}| > \Delta_q
\end{aligned}$$

or, more precisely,

$$\begin{aligned}
&\int_{|\mathbf{p}'-\mathbf{p}|>\Delta_p} d^3\mathbf{p}\int_{|\mathbf{q}'-\mathbf{q}|>\Delta_q} d^3\mathbf{q}\rho(\mathbf{p},\mathbf{q},s)e^{-[(\mathbf{p}-\mathbf{p}')/2\Delta_p]^2} \\
&\quad\times e^{-[(\mathbf{q}-\mathbf{q}')/2\Delta_q]^2} \approx 0.
\end{aligned}$$

In Appendix B, we show that condition (29) is satisfied when for the considered density matrix $\bar{D}_1$, the parameter Δ can be chosen such that

$$\left|\left(\frac{\partial}{\partial z}\right)^n p(z,s)\right| < \infty, \quad n = 1,\ldots,n_{\max},$$

$$\left|\left(\frac{\partial}{\partial z}\right)^n p(z,s)\right| \approx 0, \quad n > n_{\max}.$$

For the following considerations, we will assume

$$n_{\max} = 2, \tag{30}$$

which implies that on the scale of $\Delta_q = \Delta$ and Δ_p, the function $\rho(\mathbf{p},\mathbf{q},s)$ depends only weakly on its arguments.[19] Then, due to the presence of the overlap function $|\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle|^2$ under the integrals, we can approximate the function $\rho(\mathbf{p}',\mathbf{q}',s)$ by

$$\begin{aligned}
\rho(\mathbf{p}',\mathbf{q}',s) \approx \rho(\mathbf{p},\mathbf{q},s) &+ (\mathbf{p}'-\mathbf{p})\cdot\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} \\
&+ (\mathbf{q}'-\mathbf{q})\cdot\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}.
\end{aligned} \tag{31}$$

By inserting the expression for the overlap function Eq. (18), we find that the expectation value Eq. (28) can be expressed in terms of the following integrals

$$\frac{2}{(2\pi\hbar)^3}\int_{\mathbb{R}^3} d^3\mathbf{q}' e^{i\mathbf{k}\cdot(\mathbf{q}+\mathbf{q}')/2}e^{-[(\mathbf{q}'-\mathbf{q})/2\Delta]^2}\int_{\mathbb{R}^3} d^3\mathbf{p}' e^{-[(\mathbf{p}'-\mathbf{p})\Delta/\hbar]^2}\sinh\left(\frac{\Delta^2\mathbf{k}\cdot(\mathbf{p}'-\mathbf{p})}{\hbar}\right)\begin{cases}1 & \text{(a)}\\ (\mathbf{p}'-\mathbf{p}) & \text{(b)}\\ (\mathbf{q}'-\mathbf{q}) & \text{(c)}.\end{cases}$$

Clearly, contributions (a) and (c) are equal to zero since the integrand is antisymmetric with respect to $\mathbf{p}'-\mathbf{p}$. The remaining term (b) can be rewritten in the following form:

$$\frac{2}{(2\pi\hbar)^3}e^{i\mathbf{k}\cdot\mathbf{q}}\int_{\mathbb{R}^3} d^3\mathbf{q}' e^{i\mathbf{k}\cdot\mathbf{q}'/2}e^{-\mathbf{q}'^2/4\Delta^2}\int_{\mathbb{R}^3} d^3\mathbf{p}' e^{-\mathbf{p}'^2\Delta^2/\hbar^2}\sinh\left(\frac{\Delta^2\mathbf{k}\cdot\mathbf{p}'}{\hbar}\right)\mathbf{p}' = e^{i\mathbf{k}\cdot\mathbf{q}}\hbar\mathbf{k},$$

so that we finally get

$$\langle z,s|\frac{i}{\hbar}[\bar{D}_1,V(\mathbf{Q})]|z,s\rangle$$
$$=\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}\cdot\left(\frac{i}{\hbar}\int_{\mathbb{R}^3}d^3\mathbf{k}\hat{V}(\mathbf{k})e^{-\Delta^2\mathbf{k}^2/2}e^{i\mathbf{k}\cdot\mathbf{q}}\hbar\mathbf{k}\right)$$
$$=\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}\cdot\left(\int_{\mathbb{R}^3}d^3\mathbf{k}(i\mathbf{k})\hat{V}(\mathbf{k})e^{-\Delta^2\mathbf{k}^2/2}e^{i\mathbf{k}\cdot\mathbf{q}}\right)$$
$$=\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}\cdot\frac{\partial V^c(\mathbf{q})}{\partial\mathbf{q}},\tag{32}$$

where we used Eq. (27) in the last line.

Let us now evaluate the remaining expectation values $\langle z,s|\frac{i}{\hbar}[\bar{D}_1,T]|z,s\rangle$. By using Eq. (A29) and the commutation relations Eq. (A5), the kinetic-energy operator can be rewritten as

$$T=\frac{\mathbf{P}^2}{2m}=\frac{\hbar^2}{4\Delta^2}[(\mathbf{A}^\dagger)^2+\mathbf{A}\cdot\mathbf{A}^\dagger+\mathbf{A}^\dagger\cdot\mathbf{A}+\mathbf{A}^2]$$
$$=\frac{\hbar^2}{4\Delta^2}[(\mathbf{A}^\dagger)^2+3+2\mathbf{A}^\dagger\cdot\mathbf{A}+\mathbf{A}^2]=\frac{\hbar^2}{4\Delta^2}[(\mathbf{A}^\dagger+\mathbf{A})^2+3].$$

From Eqs. (A28) and (10), we get

$$\langle\mathbf{p},\mathbf{q},s|T|\mathbf{p}',\mathbf{q}',s'\rangle$$
$$=\delta_{ss'}\frac{\hbar^2}{2m}\frac{1}{4\Delta^2}[(\boldsymbol{\alpha}^\star+\boldsymbol{\alpha}')^2+3]\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle$$
$$=\frac{\hbar^2}{2m}\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle\left[\left(\frac{\mathbf{p}+\mathbf{p}'}{2\hbar}\right)^2-\left(\frac{\mathbf{q}-\mathbf{q}'}{4\Delta^2}\right)^2\right.$$
$$\left.+\frac{i(\mathbf{p}+\mathbf{p}')\cdot(\mathbf{q}'-\mathbf{q})}{4\Delta^2\hbar}+\frac{3}{4\Delta^2}\right].\tag{33}$$

The last line implies

$$\langle\mathbf{p},\mathbf{q},s|T|\mathbf{p},\mathbf{q},s\rangle=\frac{1}{2m}\left(\mathbf{p}^2+\frac{3\hbar^2}{4\Delta^2}\right).$$

With Eqs. (20), (31), and (33), the expectation value of the commutator can be written in the following form:

$$\langle\mathbf{p},\mathbf{q},s|\frac{i}{\hbar}[\bar{D}_1,T]|\mathbf{p},\mathbf{q},s\rangle$$
$$=\frac{i}{\hbar}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6}d^3\mathbf{p}'d^3\mathbf{q}'\rho(\mathbf{p}',\mathbf{q}',s)(\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle\langle\mathbf{p}',\mathbf{q}',s|T|\mathbf{p},\mathbf{q},s\rangle-\langle\mathbf{p},\mathbf{q},s|T|\mathbf{p}',\mathbf{q}',s\rangle\langle\mathbf{p}',\mathbf{q}',s|\mathbf{p},\mathbf{q},s\rangle)$$
$$=\frac{i}{\hbar}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6}d^3\mathbf{p}'d^3\mathbf{q}'\rho(\mathbf{p}',\mathbf{q}',s)|\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle|^2\frac{\hbar^2}{2m}\left(\frac{2i(\mathbf{p}+\mathbf{p}')\cdot(\mathbf{q}'-\mathbf{q})}{4\Delta^2\hbar}\right)$$
$$=\frac{1}{4m\Delta^2}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6}d^3\mathbf{p}'d^3\mathbf{q}'\rho(\mathbf{p}',\mathbf{q}',s)e^{-[(\mathbf{q}'-\mathbf{q})/2\Delta]^2}e^{-[(\mathbf{p}'-\mathbf{p})\Delta/\hbar]^2}(\mathbf{p}+\mathbf{p}')\cdot(\mathbf{q}-\mathbf{q}').$$

By using, again, the approximation equation (31), we are left with the following integrals:

$$\frac{1}{4m\Delta^2}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6}d^3\mathbf{p}'d^3\mathbf{q}'e^{-[(\mathbf{q}'-\mathbf{q})/2\Delta]^2}e^{-[(\mathbf{p}'-\mathbf{p})\Delta/\hbar]^2}(\mathbf{p}+\mathbf{p}')\cdot(\mathbf{q}-\mathbf{q}')\begin{cases}1 & \text{(a)}\\(\mathbf{p}'-\mathbf{p}) & \text{(b)}\\(\mathbf{q}'-\mathbf{q}) & \text{(c)}.\end{cases}$$

By inspecting the symmetry of the integrands, we see that integrals (a) and (b) are zero. We are thus left with integral (c), which is equal to $-\frac{\mathbf{p}}{m}$, so that, finally,

$$\langle\mathbf{p},\mathbf{q},s|\frac{i}{\hbar}[\bar{D}_1,T]|\mathbf{p},\mathbf{q},s\rangle=-\frac{\mathbf{p}}{m}\cdot\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}.\tag{34}$$

B. Phase-space representation of the superoperator Γ

The last term in Eq. (9) expresses the action of the linear superoperator, $\Gamma(t)\in\mathcal{L}[\mathcal{L}(\mathcal{H})]$, on $\bar{D}_1(t)\in\mathcal{L}(\mathcal{H})$. In our derivation of the master equations, this superoperator was defined in terms of its matrix elements $\Gamma^{\kappa\lambda}_{\nu\mu}(t)$ in the basis of the eigenstates $|\nu\rangle$, $|\mu\rangle$, $|\kappa\rangle$, $|\lambda\rangle$ of the one-particle operator $\hat{H}_0^{(1)}$ [see Eq. (5)]. By remembering that the coherent states satisfy closure relation (A38), the above relation can be im-

mediately rewritten in terms of coherent states, where it reads as

$$\langle \boldsymbol{u}|\Gamma(Y)|\boldsymbol{u}'\rangle = \int_{\mathcal{A}} d\boldsymbol{u}'' \int_{\mathcal{A}} d\boldsymbol{u}''' \Gamma(\boldsymbol{u},\boldsymbol{u}';\boldsymbol{u}'',\boldsymbol{u}''') \times \langle \boldsymbol{u}''|Y|\boldsymbol{u}'''\rangle, \quad \forall \ Y \in \mathcal{L}(\mathcal{H}), \tag{35}$$

where

$$\Gamma(\boldsymbol{u},\boldsymbol{u}';\boldsymbol{u}'',\boldsymbol{u}''') = \sum_{\nu\mu\kappa\lambda} \langle \boldsymbol{u}''|\kappa\rangle\langle \boldsymbol{u}|\nu\rangle \Gamma^{\kappa\lambda}_{\nu\mu} \langle \lambda|\boldsymbol{u}'''\rangle\langle \mu|\boldsymbol{u}'\rangle.$$

Written in the explicit form of Eq. (35), the second term in Eq. (23) reads as

$$\langle z,s|\Gamma[\bar{D}_1(t)]|z,s\rangle = \sum_{s'} \int_{\mathbb{R}^6} d^6z' \int_{\mathbb{R}^6} d^6z'' \langle z',s'|\bar{D}_1(t)|z'',s'\rangle \times \Gamma[(z,s),(z,s);(z',s'),(z'',s')].$$

The above expectation value describes the influence of the electron-electron interaction, as well as that of the electron-bath interactions on the evolution of $\langle z,s|\bar{D}_1(t)|z,s\rangle$. It corresponds to the "collision term" in the Boltzmann description of a classical gas.

After insertion of results (32) and (34) and Eq. (24) into the master equations in Eq. (23) and by using, again, the diagonal representation of the one-particle density matrix Eq. (20), which yields

$$\langle z',\boldsymbol{s}'|\bar{D}_1(t)|z'',s'\rangle = \int_{\mathbb{R}^6} dz \rho(z,s')\langle z',\boldsymbol{s}'|z,s'\rangle\langle z,s'|z'',\boldsymbol{s}'\rangle, \tag{36}$$

we obtain the quantum-Boltzmann equation expressed in the generating system of coherent states:

$$\begin{aligned}\int_{\mathbb{R}^6} dz' g(z,z') \frac{d\rho(z',s)}{dt} &= \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}} \cdot \frac{\partial \rho(\mathbf{p},\mathbf{q},s)}{\partial \mathbf{p}} - \frac{\mathbf{p}}{m} \cdot \frac{\partial \rho(\mathbf{p},\mathbf{q},s)}{\partial \mathbf{q}} \\ &+ \sum_{s'} \int_{\mathbb{R}^6} dz' \int_{\mathbb{R}^6} dz'' \Gamma[(z,s),(z,s);(z',s'),(z'',s')] \\ &\times \int_{\mathbb{R}^6} dz''' \rho(z''',s')\langle z',s'|z''',s'\rangle\langle z''',s'|z'',s'\rangle. \end{aligned} \tag{37}$$

The weight function $g(z,z')$ under the integral on the left-hand side is positive and normalized to 1 [see Eqs. (16), (17), and (19)]. It becomes negligibly small for states, $|\boldsymbol{u}'\rangle = |\mathbf{p}(z'),\mathbf{q}(z'),s'\rangle$, with $|\mathbf{q}(z')-\mathbf{q}(z)| \gg \Delta_q$ and $|\mathbf{p}(z')-\mathbf{p}(z)| \gg \Delta_p$. Under conditions (29) and (30), we can therefore restrict the integration over z' to a limited region around $\mathbf{p},\mathbf{q}$.

Apart from the spin variable s, the first two terms on the right-hand side of Eq. (37) depend only on $\mathbf{p},\mathbf{q}$. They have the form of the drift and of the diffusion term in the classical Boltzmann equation. It should be kept in mind, however, that the function $\rho(\mathbf{p},\mathbf{q},s)$ does not describe a probability distribution.

The last term on the right-hand side of the master equations in Eq. (37) depends on the function $\Gamma[(z,s),(z,s);(z',s'),(z'',s')]$, which describes the influence of the electron-electron interaction and of the phonon- and photon-bath subsystems on the evolution of the electronic system. In order to understand the influence of this term, we first have to recognize that the one-particle operators, $Q^A_{j\alpha}, A^e_\alpha \in \mathcal{L}(\mathcal{H})$, entering the interaction Hamiltonian are local operators, i.e., we have

$$\langle \mathbf{p},\mathbf{q},s|A_\alpha|\mathbf{p}',\mathbf{q}',s'\rangle \cong 0 \quad \text{for } |\mathbf{q}-\mathbf{q}'| > r, \quad \forall \ \alpha$$
$$\langle \mathbf{p},\mathbf{q},s|Q^A_{j\alpha}|\mathbf{p}',\mathbf{q}',s'\rangle \cong 0 \quad \text{for } |\mathbf{q}-\mathbf{q}'| > r, \quad \forall \ j,\alpha.$$

The range r fixes the maximum spatial range of the interaction Hamiltonians, including the electron-electron interaction. In most cases, it will not be of interest to work with coherent states that decay on a scale much shorter or much longer than r along the $\mathbf{q}$ directions. For the following discussions, we will thus suppose that

$$r \approx \Delta_q.$$

Let us recall that the Γ term represents contributions of second order in the interaction (see Ref. 14), so that the function $\Gamma[(z,s),(z,s);(z',s'),(z'',s')]$ gives only significant contributions when the overlaps in real space between coherent states $|z\rangle$ and $|z'\rangle$ and also with $|z''\rangle$ become important. Thus, the integrations in the third term on the right-hand side of Eq. (37) can be restricted to z' and z'', with the following:

$$|\mathbf{q}(z')-\mathbf{q}(z)| \le 2r, \quad |\mathbf{q}(z'')-\mathbf{q}(z)| \le 2r, \tag{38}$$

which implies

$$|\mathbf{q}(z')-\mathbf{q}(z'')| < 4r. \tag{39}$$

From Eqs. (38) and (39), it follows that the "final" states $|z',s'\rangle$ and $|z'',s'\rangle$ are located in the same *spatial* region as the "initial" state $|z,s\rangle$, i.e., the spatial centers $\mathbf{q}(z')$ and $\mathbf{q}(z'')$ are close to the spatial center $\mathbf{q}(z)$ of the initial state. A similar proximity condition also holds in the $\mathbf{p}$ direction. In fact, from Eq. (36) and condition (29), we find that

$$\rho(z''',s')\langle z',s'|z''',s'\rangle\langle z''',s'|z'',s'\rangle \approx 0, \tag{40}$$

for

$$\begin{aligned} |\mathbf{p}(z')-\mathbf{p}(z''')| &> 2\Delta_p, \\ |\mathbf{p}(z'')-\mathbf{p}(z''')| &> 2\Delta_p, \\ |\mathbf{q}(z')-\mathbf{q}(z''')| &> 2\Delta_q, \\ |\mathbf{q}(z'')-\mathbf{q}(z''')| &> 2\Delta_q, \end{aligned} \tag{41}$$

or

$$\begin{aligned} |\mathbf{p}(z')-\mathbf{p}(z'')| &> 4\Delta_p, \\ |\mathbf{q}(z')-\mathbf{q}(z'')| &> 4\Delta_q, \end{aligned} \tag{42}$$

where the last condition enforces condition (39). Accordingly, coherent states z', z'', z''' contributing to the third term in Eq. (37) must lie close together in phase space.

From the above considerations, it follows that, for a starting vector, $|z,s\rangle = |\mathbf{p},\mathbf{q},s\rangle$, which is defined by the left-hand

side of Eq. (37), we only need to include the contributions of vectors, $|z',s'\rangle \equiv |\mathbf{p}',\mathbf{q}',s'\rangle$ and $|z'',s'\rangle = |\mathbf{p}'',\mathbf{q}'',s'\rangle$, that are located in the same spatial neighborhood of $|\mathbf{p},\mathbf{q},s\rangle$, where the latter is defined by a sphere with a radius $4r$ centered at $\mathbf{q}$. Moreover, condition (42) implies that the final states $|z',s'\rangle$ and $|z'',s''\rangle$ contributing to this "scattering term" are also close in the $\mathbf{p}$ directions, while their distance with respect to $\mathbf{p}$ solely depends on the characteristics of the interaction Hamiltonians.

According to Eqs. (38), (39), (41), and (42), the action of the operators on the right-hand side of Eq. (37) on the function $\rho(z,s)$ characterizing the one-particle density matrix is limited to a finite region in real space. This property allows us to extend the approach to infinite systems without any difficulty. Thus, the restriction to systems with a definite number N of electrons, which was necessary in Ref. 14, is no longer required in the present phase-space formulation of the quantum-Boltzmann equation and can be dropped. Moreover, we note that, in contrast to the original derivation of Eq. (9) in Ref. 14, Eq. (37) does not depend on the existence of eigenstates of the one-particle Hamiltonian. This allows us to include external electric or magnetic fields in Eq. (37) without any difficulties and to study the associated electric currents.

We emphasize that, apart from the supposed homogeneity of the electronic system expressed by Eq. (31) and the assumption that the one-particle density matrix in its diagonal representation is described by a bounded function $\rho(z)$, we have not made any restrictive assumptions to derive Eq. (37) from the quantum-master equations in Eq. (9). Thus, provided that the above conditions are satisfied, Eq. (37) accounts for the "quantum" evolution without further restrictions.

V. CLASSICAL LIMIT

A. Quasiorthogonality in phase space and probability distributions

According to Eqs. (20) and (21), the one-particle density matrix $\bar{D}_1$ can be characterized by either the functions $p(z,s)$ or the functions $\rho(z,s)$. Both functions are related by Eq. (21). Since they satisfy the normalization condition (22), it is always possible to choose sufficiently large cell volumes Ω in phase space as in Eq. (45), so that the mean value taken over a subvolume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$ of volume Ω and centered at $\mathbf{p}_0,\mathbf{q}_0$:

$$\bar{\rho}_\Omega(\mathbf{p}_0,\mathbf{q}_0,s) = \frac{1}{\Omega}\int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q}\rho(\mathbf{p},\mathbf{q},s),$$

becomes positive. In order to show that these mean values can be interpreted as a probability associated with the subvolume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$, we consider a subvolume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$ with a volume Ω and centered at some point $\mathbf{p}_0,\mathbf{q}_0$ and define an associated weight function (or "characteristic function"):

$$\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0) = \begin{cases} \dfrac{1}{\Omega} & \text{for } \mathbf{p},\mathbf{q} \in \Omega(\mathbf{p}_0,\mathbf{q}_0) \\ 0 & \text{otherwise,} \end{cases} \tag{43}$$

which satisfies the following normalization condition:

$$\int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0) = 1. \tag{44}$$

For sufficiently large cell volumes $\Omega(\mathbf{p}_0,\mathbf{q}_0)$ with cell dimensions much larger than Δ_q in the $\mathbf{q}$ directions and Δ_p in the $\mathbf{p}$ directions, where surface contributions can be neglected, we get

$$\begin{aligned}
0 \le \bar{\rho}_\Omega(\mathbf{p}_0,\mathbf{q}_0,s) &\equiv \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0)p(\mathbf{p},\mathbf{q},s) = \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0)\langle\mathbf{p},\mathbf{q},s|\bar{D}_1|\mathbf{p},\mathbf{q},s\rangle \\
&= \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0)\rho(\mathbf{p}',\mathbf{q}',s)g(\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}') \\
&\approx \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\chi_\Omega(\mathbf{p}'-\mathbf{p}_0,\mathbf{q}'-\mathbf{q}_0)\rho(\mathbf{p}',\mathbf{q}',s)g(\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}') \\
&= \int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\chi_\Omega(\mathbf{p}'-\mathbf{p}_0,\mathbf{q}'-\mathbf{q}_0)\rho(\mathbf{p}',\mathbf{q}',s)\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}g(\mathbf{p},\mathbf{q},\mathbf{p}',\mathbf{q}') \\
&= \int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\chi_\Omega(\mathbf{p}'-\mathbf{p}_0,\mathbf{q}'-\mathbf{q}_0)\rho(\mathbf{p}',\mathbf{q}',s) \equiv \bar{\rho}_\Omega(\mathbf{p}_0,\mathbf{q}_0,s),
\end{aligned} \tag{45}$$

where the last line is obtained from Eq. (19). Thus, the average $\bar{\rho}_\Omega(\mathbf{p},\mathbf{q},s) \ge 0$ can be obtained by integrating either $p(\mathbf{p},\mathbf{q},s)$ or $\rho(\mathbf{p},\mathbf{q},s)$ over a cell Ω centered at $\mathbf{p},\mathbf{q}$ and with dimensions much larger than Δ_p and Δ_q.[20] From Eq. (22), we get

$$\int_{\mathcal{A}} d\boldsymbol{u}\rho(\boldsymbol{u}) = \frac{1}{(2\pi\hbar)^3}\sum_s \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\rho(\mathbf{p},\mathbf{q},s) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\int_{\mathbb{R}^6} d^3\mathbf{p}_0d^3\mathbf{q}_0\rho(\mathbf{p}_0,\mathbf{q}_0,s)\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0)$$

and thus,

$$\frac{1}{(2\pi\hbar)^3}\sum_s \int_{\mathbb{R}^6} d^3\mathbf{p}d^3\mathbf{q}\bar{\rho}_\Omega(\mathbf{p},\mathbf{q},s) = 1. \tag{46}$$

Clearly, the functions $\bar{\rho}_\Omega(\mathbf{p},\mathbf{q},s)$ can only be interpreted as probability distributions if the subspaces associated with the coherent states, $|\mathbf{p},\mathbf{q},s\rangle, \mathbf{p},\mathbf{q}\in\Omega(\mathbf{p}_0,\mathbf{q}_0)$ and $|\mathbf{p}',\mathbf{q}',s\rangle, \mathbf{p}',\mathbf{q}'\in\Omega_c(\mathbf{p}_0,\mathbf{q}_0)$, with

$$\Omega(\mathbf{p}_0,\mathbf{q}_0) + \Omega_c(\mathbf{p}_0,\mathbf{q}_0) = \mathbb{R}^6,$$

can be considered orthogonal. In order to see that this is the case for sufficiently large compact and convex volumes $\Omega_{(\mathbf{p}_0,\mathbf{q}_0)}$, we define the following self-adjoint operators:

$$P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} = \frac{1}{(2\pi\hbar)^3}\sum_s \int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q}|\mathbf{p},\mathbf{q},s\rangle\langle\mathbf{p},\mathbf{q},s|, \tag{47}$$

$$P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} = \frac{1}{(2\pi\hbar)^3}\sum_s \int_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q}|\mathbf{p},\mathbf{q},s\rangle\langle\mathbf{p},\mathbf{q},s|. \tag{48}$$

Both operators commute with each other. Equations (15), (47), and (48) imply

$$P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} + P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} = \mathbb{1}.$$

In order to obtain quasiorthogonal subspaces associated with the coherent states inside and outside the volume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$, we have to find the conditions under which $P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}$ and $P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)}$ can be considered to be orthogonal projectors, so that

$$(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} + P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})^2\mathcal{H} \approx (P^2_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} + P^2_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})\mathcal{H}. \tag{49}$$

The above condition requires that the Hilbert–Schmidt scalar product $\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})$ is negligibly small with respect to $\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}) \ll \mathrm{Tr}(P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})$. We have

$$\begin{aligned}\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)}) &= \frac{1}{(2\pi\hbar)^6}\sum_i\sum_s \int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q}\int_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}'d^3\mathbf{q}'\langle i|\mathbf{p},\mathbf{q},s\rangle\langle\mathbf{p},\mathbf{q},s|\mathbf{p}',\mathbf{q}',s\rangle\langle\mathbf{p}',\mathbf{q}',s|i\rangle \\ &= \frac{1}{(2\pi\hbar)^6}\sum_s \int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q}\int_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}'d^3\mathbf{q}'|\langle\mathbf{p}',\mathbf{q}',s|\mathbf{p},\mathbf{q},s\rangle|^2,\end{aligned}$$

and accordingly,

$$\begin{aligned}&\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}) \\ &= \frac{1}{(2\pi\hbar)^6}\sum_s \int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}d^3\mathbf{q} \\ &\quad\times\int_{\Omega(\mathbf{p}_0,\mathbf{q}_0)} d^3\mathbf{p}'d^3\mathbf{q}'|\langle\mathbf{p}',\mathbf{q}',s|\mathbf{p},\mathbf{q},s\rangle|^2.\end{aligned}$$

From Eqs. (17) and (18), we see that $\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})$ has only contributions from the surface region. According to Eq. (18), the width of the contributing volume is of the order $(4\Delta_q\Delta_p)^3 = (2\hbar)^3$. The contribution to $\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})$ is thus on the order of $\approx S(2\hbar)^3$, where S denotes the surface of the volume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$. The Hilbert–Schmidt scalar product $\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)})$ has contributions from the whole volume Ω. Thus, we have

$$\frac{\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)})}{\mathrm{Tr}(P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)})} \propto \frac{S(2\hbar)^3}{\Omega} < \epsilon \ll 1. \tag{50}$$

The parameter ϵ defines the accuracy to which the subspaces of the Hilbert space generated by the coherent states centered inside or outside the volume $\Omega(\mathbf{p}_0,\mathbf{q}_0)$ may be considered to be orthogonal. It is always nonzero, but it may be chosen to be arbitrarily small. A small ϵ corresponds to large volumes Ω. The quasiorthogonality of the following subspaces:

$$\mathcal{H}_{\Omega_{(\mathbf{p}_0,\mathbf{q}_0)}} = P_{\Omega(\mathbf{p}_0,\mathbf{q}_0)}\mathcal{H}$$

and

$$\mathcal{H}_{\Omega_{c(\mathbf{p}_0,\mathbf{q}_0)}} = P_{\Omega_c(\mathbf{p}_0,\mathbf{q}_0)}\mathcal{H}$$

expressed by Eqs. (49) and (50), put together with Eqs. (45) and (46), finally allows us to interpret $\bar{\rho}_\Omega(\mathbf{p},\mathbf{q},s)\geq 0$ as a probability density in phase space at $(\mathbf{p},\mathbf{q})$, which describes the distribution of electrons with spin s on the scale of the volume Ω.

In Sec. V, we will show that starting from the quantum-Boltzmann equation in phase space [Eq. (37)], one can finally derive the semi-classical Boltzmann equation, which describes the large scale evolution of the electron gas in a solid.

B. Semi-classical Boltzmann equation

In Sec. V A, we have seen that the averaging over a sufficiently large volume Ω to satisfy the condition Eq. (50)

allows us to interpret the averaged function $\bar{\rho}_\Omega(\mathbf{p},\mathbf{q})$ as a probability distribution [see also Eq. (45)]. Clearly, this is a necessary prerequisite for the classical Boltzmann equation. By using the characteristic function defined in Eqs. (43) and (44), we thus define the following probability:

$$\bar{\rho}_\Omega(\mathbf{p},\mathbf{q},s) = \int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\,\chi_\Omega(\mathbf{p}-\mathbf{p}',\mathbf{q}-\mathbf{q}')\rho(\mathbf{p}',\mathbf{q}',s)$$

$$\approx \frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\rho(\mathbf{p}',\mathbf{q}',s) \geq 0, \tag{51}$$

where the phase-space volume $\Omega(\mathbf{p},\mathbf{q})$ with volume Ω is centered at $\mathbf{p},\mathbf{q}$. In the following, we will omit the index Ω, i.e., we replace $\bar{\rho}_\Omega$ by $\bar{\rho}$. According to Eq. (45), we get the following for the average of the left-hand side of Eq. (37) taken over the volume $\Omega(\mathbf{p},\mathbf{q})$:

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\frac{d\rho(\mathbf{p}',\mathbf{q}',s)}{dt} = \frac{d\bar{\rho}(\mathbf{p},\mathbf{q},s)}{dt}. \tag{52}$$

Some additional approximations are necessary if we want to express the right-hand side of Eq. (37) in terms of $\bar{\rho}(\mathbf{p},\mathbf{q},s)$. For the first term, we have to assume that the force $\frac{\partial V^c(\mathbf{q}')}{\partial \mathbf{q}'}$ does not significantly vary over the integration domain in the $\mathbf{q}$ subspace and that

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\frac{\partial\rho(\mathbf{p}',\mathbf{q}',s)}{\partial\mathbf{p}'} \approx \frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}. \tag{53}$$

Then, this term becomes

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\frac{\partial V^c(\mathbf{q}')}{\partial\mathbf{q}'}\cdot\frac{\partial\rho(\mathbf{p}',\mathbf{q}',s)}{\partial\mathbf{p}'}$$

$$\approx \frac{\partial V^c(\mathbf{q})}{\partial\mathbf{q}}\cdot\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}. \tag{54}$$

For the second term on the right-hand side of Eq. (37), we have to calculate the following average:

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\mathbf{p}'\cdot\frac{\partial\rho(\mathbf{p}',\mathbf{q}',s)}{\partial\mathbf{q}'}.$$

By recognizing that $\mathbf{p}$ is the average value of $\mathbf{p}'$ in the integration domain, we can approximate the mean value of the product by the product of the mean values,[21] i.e.,

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\mathbf{p}'\cdot\frac{\partial\rho(\mathbf{p}',\mathbf{q}',s)}{\partial\mathbf{q}'} \approx \mathbf{p}\cdot\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}. \tag{55}$$

Let us now consider the remaining collision term in Eq. (37). In the classical Boltzmann approach, the following conditions:

$$\Gamma[(z,s),(z,s);(z',s'),(z'',s')] \cong 0 \quad \text{if } \mathbf{q}(z'),\mathbf{q}(z'')\notin\Omega(\mathbf{p},\mathbf{q})\equiv\Omega(z), \tag{56}$$

$$\Gamma[(z,s),(z,s);(z',s'),(z'',s')] \cong 0 \quad \text{if } \mathbf{p}(z'),\mathbf{p}(z'')\in\Omega(\mathbf{p},\mathbf{q}) \tag{57}$$

have to be satisfied. This can be achieved by an adequate choice of the free parameters Δ_q, $d_q \gg \Delta_q$, and $d_p \gg \Delta_p$, where the parameters d_q and d_p characterize the dimensions of the subvolume Ω that is covered by the characteristic function $\chi_\Omega(\mathbf{p}-\mathbf{p}_0,\mathbf{q}-\mathbf{q}_0)$ introduced in Eqs. (43) and (44). Having specified the parameter Δ_q entering the definitions of the coherent states, we can investigate the behavior of the functions $\Gamma[(z,s),(z,s);(z',s'),(z'',s')]$ in phase space. We then look for the smallest dimensions d_q and d_p of the subvolume $\Omega = d_q^3 d_p^3$ entering the definition of the characteristic function, which allow us to satisfy the quasiorthogonality condition Eq. (50). In addition, the interaction radius $4r$ [see Eqs. (38) and (39)] must be much smaller than d_q. Consequently, the cell dimensions d_q and d_p must satisfy the conditions $d_q \gg 4r \gg \Delta_q$ and $d_p \gg \Delta_p$. The choice $d_q \gg \Delta_q$ is also optimal to satisfy condition (56). In order to also satisfy condition (57), which guarantees that scattering within the cell $\Omega(\mathbf{p},\mathbf{q})$ can be neglected, we choose the smallest parameter d_p that is still compatible with condition (50).

After the above considerations, we are now prepared to discuss the contribution of the collision term in the classical limit. Explicitly written, it reads as

$$\frac{1}{\Omega}\sum_{s'}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\int_{\mathbb{R}^6} dz''\int_{\mathbb{R}^6} dz'''\Gamma[(\mathbf{p}',\mathbf{q}',s),(\mathbf{p}',\mathbf{q}',s);(z'',s'),(z''',s')]\int_{\mathbb{R}^6} dz''''\rho(z'''',s')\langle z''|z''''\rangle\langle z''''|z'''\rangle$$

$$= \sum_{s'}\int_{\mathbb{R}^6} dz''\int_{\mathbb{R}^6} dz'''\left\{\frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\Gamma[(\mathbf{p}',\mathbf{q}',s),(\mathbf{p}',\mathbf{q}',s);(z'',s'),(z''',s')]\right\}\int_{\mathbb{R}^6} dz''''\rho(z'''',s')\langle z''|z''''\rangle\langle z''''|z'''\rangle$$

$$= \sum_{s'}\int_{\mathbb{R}^6} dz''\int_{\mathbb{R}^6} dz'''\bar{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'',s'),(z''',s')]\int_{\mathbb{R}^6} dz''''\rho(z'''',s')\langle z''|z''''\rangle\langle z''''|z'''\rangle$$

$$= \sum_{s'}\int_{\mathbb{R}^6} dz''''\rho(z'''',s')\int_{\mathbb{R}^6} dz''\int_{\mathbb{R}^6} dz'''\bar{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'',s'),(z''',s')]\langle z''|z''''\rangle\langle z''''|z'''\rangle, \tag{58}$$

where $\bar{\Gamma}((\mathbf{p},\mathbf{q},s);(z'',s'),(z''',s'))$ denotes the following average:

$$\bar{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'',s'),(z''',s')] = \frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\Gamma[(\mathbf{p}',\mathbf{q}',s),(\mathbf{p}',\mathbf{q}',s);(z'',s'),(z''',s')].$$

With

$$\hat{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'''',s')] = \int_{\mathbb{R}^6} dz'' \int_{\mathbb{R}^6} dz''' \bar{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'',s'),(z''',s')]\langle z''|z''''\rangle\langle z''''|z'''\rangle, \tag{59}$$

Eq. (58) becomes

$$\frac{1}{\Omega}\sum_{s'}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}'d^3\mathbf{q}'\int_{\mathbb{R}^6} dz''\int_{\mathbb{R}^6} dz'''\Gamma[(\mathbf{p}',\mathbf{q}',s),(\mathbf{p}',\mathbf{q}',s);(z'',s'),(z''',s')]\int_{\mathbb{R}^6} dz''''\rho(z'''',s')\langle z''|z''''\rangle\langle z''''|z'''\rangle$$

$$= \sum_{s'}\int_{\mathbb{R}^6} dz''''\hat{\Gamma}[(\mathbf{p},\mathbf{q},s);(z'''',s')]\rho(z'''',s') \approx \sum_{s'}\int_{\mathbb{R}^6} dz'\overline{\hat{\Gamma}[(\mathbf{p},\mathbf{q},s),(z',s')]}\bar{\rho}(z',s'), \tag{60}$$

where in the last line, we have replaced the function $\rho(z',s')$ by its average $\bar{\rho}(z',s')$ taken over a volume $\Omega(\mathbf{q},\mathbf{p}')$ and where in the spirit of Eq. (50), the functions $|z''\rangle \in \Omega(\mathbf{q},\mathbf{p}')$ can be considered to be practically orthogonal to the functions $|z'\rangle \in \Omega(\mathbf{q},\mathbf{p})$. In this case, following the procedure leading to Eq. (45), the resulting positive function $\bar{\rho}(z',s')$ can be interpreted as a probability density that characterizes the electron distribution in the region $\Omega(\mathbf{q},\mathbf{p}')$. The function $\overline{\hat{\Gamma}[(\mathbf{p},\mathbf{q},s),\mathbf{z}',s']}$ describes the corresponding average of on $\hat{\Gamma}[(\mathbf{p},\mathbf{q},s),\mathbf{z}''',s']$ with respect to z''' over the volume $\Omega(\mathbf{q},\mathbf{p}')$.[22] With Eqs. (54), (55), and (60), and the averaging procedure (51) we finally obtain from Eq. (37) the following master equation:

$$\frac{d\bar{\rho}(\mathbf{p},\mathbf{q},s)}{dt} = \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}}\cdot\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} - \frac{\mathbf{p}}{m}\cdot\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}$$

$$+ \frac{1}{(2\pi\hbar)^3}\sum_{s'}\int_{\mathbb{R}^6} d^3\mathbf{p}'d^3\mathbf{q}'\bar{\bar{\Gamma}}[(\mathbf{p},\mathbf{q},s);(\mathbf{p}',\mathbf{q},s')]$$

$$\times\bar{\rho}(\mathbf{p}',\mathbf{q}',s'), \tag{61}$$

where

$$\bar{\bar{\Gamma}}[(\mathbf{p},\mathbf{q},s);(\mathbf{p}',\mathbf{q},s')] = \frac{1}{\Omega}\int_{\Omega(\mathbf{p},\mathbf{q})} d^3\mathbf{p}''d^3\mathbf{q}''\overline{\hat{\Gamma}[(\mathbf{p}'',\mathbf{q}'',s),(\mathbf{z}',s')]}.$$

Equation (61) represents the classical Boltzmann equation for the evolution of the probability density $\bar{\rho}(\mathbf{p},\mathbf{q},s)$. The three terms on the right-hand side are commonly denoted as the field, diffusion, and collision terms.

VI. DISCUSSION AND CONCLUSIONS

The principal aim of our present work was to establish a link between the quantum-statistical description of a fermionic system and the corresponding semi-classical Boltzmann equation. Starting from quantum-Boltzmann equation (4), which was derived in Ref. 14 and describes the evolution of the one-particle density matrix for a many-electron system, we have studied the correspondent evolution of the electronic system in the one-particle phase space. The phase-space formulation, which constitutes the natural starting point for a comparison between the classical and the quantum descriptions, was obtained by expressing Eq. (4) in terms of the generating set of coherent states. The properties of the coherent states are presented in Appendix A. Let us resume here the most important ones, which are essential for the reformulation of the master equations. First of all, by saturating the Heisenberg inequalities [see Eq. (11)], coherent states are optimally localized in phase space. Moreover, by applying generalized translation operators Eq. (A17) in the one-particle phase space on a coherent state located at the origin, one can generate coherent states centered at arbitrary points in phase space [see Eq. (A25)]. The ensemble of these states constitutes a nonorthogonal and overcomplete generating set of the one-particle Hilbert space $\mathcal{H}$. The most important property of coherent states is that, although forming an overcomplete set, they still obey the generalized closure relation Eq. (A38). This allows us to decompose the one-particle states on the set of coherent states. Another important feature of the coherent states, which again is related to their overcompleteness, is that, according to Eq. (A42), a one-particle operator written in this nonorthogonal generating set is already completely determined by its expectation values for all coherent states. By using the last two properties, we have rewritten the quantum-Boltzmann equation in the form of Eq. (37), which is the ideal point of departure to study the evolution of the electronic system in phase space. The immediate interest of this reformulation is that, in contrast to the original formulation of the master equation, it allows us to exploit the local character of the interactions with the bath subsystems. Thus, by making a judicious

choice of the parameters defining the extension of the coherent states in the position and momentum directions, one may easily focus on physically relevant length scales, which depend on the given sample dimensions, the range of interactions, as well as on the statistical state of the system.

In the final step, we have obtained the semi-classical Boltzmann equation Eq. (61) via an additional coarse-graining procedure in phase space. For this procedure, we have exploited the quasiorthogonality between the one-particle Hilbert subspace that is generated by coherent states centered at points within a sufficiently large compact and convex subvolume $\Omega(\mathbf{p},\mathbf{q})$ in phase space and the "complementary" Hilbert subspace generated by coherent states centered outside $\Omega(\mathbf{p},\mathbf{q})$. After averaging over such volumes of size Ω, we obtain the semi-classical description of the evolution of the electron gas in phase space. The averaging (or "coarse-graining") procedure requires that the interaction of the electron gas and the bath subsystems is local in real space. Clearly, by covering the full range of physical situations in metallic systems, our approach allows us to delimit the validity range of the semi-classical description.

The original derivation of the quantum-Boltzmann equation in Ref. 14 was made for spatially confined electronic systems with a fixed number of electrons. This restriction, which was necessary to specify the one-particle Hilbert space, hindered us from describing infinite electronic systems in this approach and to treat grand-canonical ensembles. Thus, it does not allow the description of grand-canonical ensembles or reservoirs in the Landauer dc-transport theory.[9,12,13] It is thus worthwhile to realize that the above-mentioned quasiorthogonality over large distances in phase space, together with the local character of the interactions between the electron gas and the bath subsystems, allows us to extend the approach to infinite systems without any difficulty. Accordingly, the limitation to systems with a definite number N of electrons is no longer necessary in the phase-space reformulation of the quantum-Boltzmann equation. In the same spirit, one can include external electric or magnetic fields, leading to electric currents. The advantages of the phase-space formulation can thus be summarized as follows:

(i) It enables us to describe and to understand the *local evolution* of the one-particle density matrix.

(ii) It allows us to describe the evolution of the one-particle density matrix for a grand-canonical ensemble and to include external electric and magnetic fields.

(iii) In the stationary nonequilibrium case, the above-mentioned locality of the evolution justifies the introduction of the concept of *local equilibria* associated with *local chemical potentials*, which is convenient for describing the situation of dc electronic transport, e.g., in the Landauer transport theory.[9,12,13]

Finally, our derivation of the semi-classical Boltzmann equation clearly shows that the semi-classical description is not in conflict with the nonseparability of quantum states (see Refs. 1–5) and that for macroscopic systems, a classical description always becomes possible on sufficiently large scales in phase space.

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APPENDIX A: COHERENT STATES, A SHORT SUMMARY

Starting from the momentum and position operators $\mathbf{P}=(P_1,P_2,P_3)$ and $\mathbf{Q}=(Q_1,Q_2,Q_3)$, which satisfy the following commutation relations:

$$[P_k,Q_l]=-i\hbar\delta_{kl}\mathbb{1}, \quad k,l=1,2,3, \tag{A1}$$

we define the operator $\mathbf{A}=(A_1,A_2,A_3)$ and its adjoint $\mathbf{A}^\dagger=(A_1^\dagger,A_2^\dagger,A_3^\dagger)$, where the operators $A_k, k=1,2,3$ are given by

$$A_k=\frac{\Delta_q P_k - i\Delta_p Q_k}{\hbar}, \tag{A2}$$

$$A_k^\dagger=\frac{\Delta_q P_k + i\Delta_p Q_k}{\hbar}, \tag{A3}$$

and where

$$\Delta_p\Delta_q=\frac{\hbar}{2}. \tag{A4}$$

From the commutation relations Eq. (A1), we obtain

$$[A_k,A_l^\dagger]=\delta_{kl}\mathbb{1}, \quad k,l=1,2,3,$$

$$[A_k,A_l]=0, \quad [A_k^\dagger,A_l^\dagger]=0. \tag{A5}$$

By definition, the coherent state $|\mathbf{w},\mathbf{a}\rangle$ with $\mathbf{w}=\mathbf{0}$ and $\mathbf{a}=\mathbf{0}$ is an eigenvector of the operator $\mathbf{A}$ with zero eigenvalue, i.e., we have

$$A_k|\mathbf{0},\mathbf{0}\rangle=\mathbf{0}, \quad k=1,2,3. \tag{A6}$$

The eigenvectors of the following self-adjoint operator:

$$N=\mathbf{A}^\dagger\cdot\mathbf{A}=\sum_{k=1}^{3}A_k^\dagger A_k\equiv\sum_{k=1}^{3}N_k \tag{A7}$$

form a complete orthonormal basis in the one-particle Hilbert space $\mathcal{H}$. N has discrete eigenstates, which can be generated from the coherent state $|\mathbf{0},\mathbf{0}\rangle$. In order to prove this, we start from the following commutation relations:

$$[N,A_k]=-A_k, \tag{A8}$$

$$[N,A_k^\dagger]=A_k^\dagger, \tag{A9}$$

which directly follow from Eq. (A5). Let us denote the eigenvectors of the operator N by $|\mathbf{n}\rangle\equiv|n_1,n_2,n_3\rangle$ and the corresponding eigenvalue by $n=n_1+n_2+n_3$, so that

$$N|n_1,n_2,n_3\rangle=n|n_1,n_2,n_3\rangle. \tag{A10}$$

From Eqs. (A8) and (A10), we get

$$\begin{aligned}NA_k|n_1,n_2,n_3\rangle&=A_kN|n_1,n_2,n_3\rangle-A_k|n_1,n_2,n_3\rangle\\&=(n-1)A_k|n_1,n_2,n_3\rangle,\end{aligned} \tag{A11}$$

i.e., $A_k|n_1,n_2,n_3\rangle$ is an eigenvector of N with the following norm:

$$\|A_k|n_1,n_2,n_3\rangle\|^2 = \langle n_1,n_2,n_3|A_k^\dagger A_k|n_1,n_2,n_3\rangle = n_k \geq 0. \tag{A12}$$

Similarly, Eq. (A9) leads to

$$\begin{aligned} NA_k^\dagger|n_1,n_2,n_3\rangle &= A_k^\dagger N|n_1,n_2,n_3\rangle + A_k^\dagger|n_1,n_2,n_3\rangle \\ &= (n+1)A_k^\dagger|n_1,n_2,n_3\rangle. \end{aligned} \tag{A13}$$

Thus, if $|\mathbf{n}\rangle = |n_1,n_2,n_3\rangle$ is an eigenvector of N with eigenvalue n, $A_k^\dagger|\mathbf{n}\rangle$ is also an eigenvector $|\mathbf{n}+\mathbf{e}_k\rangle$ with eigenvalue $n+1$, where $\mathbf{e}_k$ is the unit vector in the k direction. Equation (A12) shows that all eigenvalues must be positive or zero. Furthermore, Eq. (A6) implies that $|0,0,0\rangle$ is an eigenvector with eigenvalue zero. The state $|0,0,0\rangle$ can thus be identified with the state $|\mathbf{0},\mathbf{0}\rangle$ in Eq. (A6). All other mutually orthogonal eigenvectors can then be generated from $|0,0,0\rangle$. We obtain

$$|n_1,n_2,n_3\rangle = d_{n_1,n_2,n_3}(A_1^\dagger)^{n_1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle. \tag{A14}$$

The constant d_{n_1,n_2,n_3} can be used to obtain normalized eigenvectors $|n_1,n_2,n_3\rangle$. From the commutation relations (A5), definition (A7) and Eqs. (A13) and (A14), we get

$$\begin{aligned} &\langle n_1,n_2,n_3|n_1',n_2',n_3'\rangle \\ &\quad = d_{n_1,n_2,n_3}^2\langle 0,0,0|(A_1)^{n_1}(A_2)^{n_2}(A_3)^{n_3} \\ &\qquad \times (A_1^\dagger)^{n_1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle\delta_{\mathbf{nn}'} \\ &\quad = d_{n_1,n_2,n_3}^2(n_1!\,n_2!\,n_3!)\delta_{\mathbf{nn}'} \equiv \delta_{\mathbf{nn}'}. \end{aligned}$$

Accordingly, the normalized eigenvectors of N are given by

$$|n_1,n_2,n_3\rangle = \frac{1}{\sqrt{n_1!\,n_2!\,n_3!}}(A_1^\dagger)^{n_1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle. \tag{A15}$$

Equations (A13) or Eq. (A12) implies

$$A_k^\dagger A_k|\mathbf{n}\rangle = n_k|\mathbf{n}\rangle. \tag{A16}$$

By using the above identity, as well as the commutation relations in Eq. (A5), we get

$$\begin{aligned} A_1|n_1,n_2,n_3\rangle &= \frac{1}{\sqrt{n_1!\,n_2!\,n_3!}}(A_1A_1^\dagger) \\ &\quad \times (A_1^\dagger)^{n_1-1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle \\ &= \frac{1}{\sqrt{n_1!\,n_2!\,n_3!}}(\mathbb{1}+A_1^\dagger A_1) \\ &\quad \times (A_1^\dagger)^{n_1-1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle \\ &= \frac{1+n_1-1}{\sqrt{n_1!\,n_2!\,n_3!}}(A_1^\dagger)^{n_1-1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle \\ &= \frac{\sqrt{n_1}}{\sqrt{(n_1-1)!\,n_2!\,n_3!}}(A_1^\dagger)^{n_1-1}(A_2^\dagger)^{n_2}(A_3^\dagger)^{n_3}|0,0,0\rangle \\ &= \sqrt{n_1}|n_1-1,n_2,n_3\rangle. \end{aligned}$$

The same calculations can be performed for the remaining operators A_2, A_3, so that

$$A_k|\mathbf{n}\rangle = \sqrt{n_k}|\mathbf{n}-\mathbf{e}_k\rangle.$$

Similarly, we find

$$A_k^\dagger|\mathbf{n}\rangle = \sqrt{n_k+1}|\mathbf{n}+\mathbf{e}_k\rangle.$$

Let us now define the translation operator:

$$T(\mathbf{w},\mathbf{a}) = e^{G(\mathbf{w},\mathbf{a})}, \tag{A17}$$

where

$$G(\mathbf{w},\mathbf{a}) = \frac{i}{\hbar}(\mathbf{w}\cdot\mathbf{Q}-\mathbf{a}\cdot\mathbf{P}). \tag{A18}$$

Equations (A17) and (A18) imply

$$T(\mathbf{w},\mathbf{a})^\dagger = T(\mathbf{w},\mathbf{a})^{-1} = T(-\mathbf{a},-\mathbf{w}).$$

From the Campbell–Baker–Hausdorff formula:

$$e^X Y e^{-X} = \sum_{n=0}^{\infty}\frac{1}{n!}\Omega_n(X,Y),$$

where

$$\Omega_n(X,Y) = [X,\Omega_{n-1}(X,Y)], \quad \Omega_0(X,Y) = Y,$$

we also obtain

$$T(\mathbf{w},\mathbf{a})^{-1}\mathbf{P}T(\mathbf{w},\mathbf{a}) = \mathbf{P}+\mathbf{w}\mathbb{1}, \tag{A19}$$

$$T(\mathbf{w},\mathbf{a})^{-1}\mathbf{Q}T(\mathbf{w},\mathbf{a}) = \mathbf{Q}+\mathbf{a}\mathbb{1}. \tag{A20}$$

The translation operators can be rewritten by using the Baker–Hausdorff theorem (see, e.g., Ref. 23),

$$e^{X+Y} = e^X e^Y e^{-(1/2)[X,Y]} = e^Y e^X e^{+(1/2)[X,Y]}.$$

For two operators X and Y satisfying the following commutation relations:

$$[X,Y] = c\mathbb{1}, \quad c\in\mathbb{C},$$

this yields

$$e^{X+Y} = e^X e^Y e^{-c/2} = e^Y e^X e^{+c/2}. \tag{A21}$$

By using the commutation relations Eq. (A1), we can thus express the translation operators defined in Eq. (A17) in the following factorized form:

$$\begin{aligned} T(\mathbf{w},\mathbf{a}) &= e^{(i/\hbar)(\mathbf{w}\cdot\mathbf{Q}-\mathbf{a}\cdot\mathbf{P})} = e^{-(i/\hbar)\mathbf{a}\cdot\mathbf{P}}e^{(i/\hbar)\mathbf{w}\cdot\mathbf{Q}}e^{(i/2\hbar)\mathbf{a}\cdot\mathbf{w}} \\ &= e^{(i/\hbar)\mathbf{w}\cdot\mathbf{Q}}e^{-(i/\hbar)\mathbf{a}\cdot\mathbf{P}}e^{-(i/2\hbar)\mathbf{a}\cdot\mathbf{w}}. \end{aligned} \tag{A22}$$

Accordingly, we have

$$\left(\mathbf{u}\cdot\frac{\partial}{\partial\mathbf{a}}\right)^n T(\mathbf{w},\mathbf{a}) = \left[\mathbf{u}\cdot\left(-\frac{i}{\hbar}\mathbf{P}+\frac{i}{\hbar}\frac{\mathbf{w}}{2}\right)\right]^n T(\mathbf{w},\mathbf{a}),$$

$$\left(\mathbf{u}\frac{\partial}{\partial\mathbf{w}}\right)^n T(\mathbf{w},\mathbf{a}) = \left[\mathbf{u}\cdot\left(\frac{i}{\hbar}\mathbf{Q}-\frac{i}{\hbar}\frac{\mathbf{a}}{2}\right)\right]^n T(\mathbf{w},\mathbf{a}),$$

where $\mathbf{u}$ is an arbitrary vector, $\mathbf{u}=(u_1,u_2,u_3)\in\mathbb{C}^3$. With Eqs. (A19) and (A20), we get

$$T(\mathbf{w},\mathbf{a})^{-1}\mathbf{A}T(\mathbf{w},\mathbf{a}) = \mathbf{A}+\boldsymbol{\alpha}\mathbb{1}, \tag{A23}$$

where

$$\boldsymbol{\alpha} = \frac{\Delta_q \mathbf{w} - i\Delta_p \mathbf{a}}{\hbar}. \tag{A24}$$

We define

$$|\mathbf{w},\mathbf{a}\rangle = T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle. \tag{A25}$$

Equation (A23) implies

$$\mathbf{A}|\mathbf{w},\mathbf{a}\rangle = \boldsymbol{\alpha}|\mathbf{w},\mathbf{a}\rangle. \tag{A26}$$

This suggests the following alternative notation:

$$|\boldsymbol{\alpha}\rangle \equiv |\mathbf{w},\mathbf{a}\rangle, \tag{A27}$$

so that Eq. (A26) becomes

$$\mathbf{A}|\boldsymbol{\alpha}\rangle = \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle. \tag{A28}$$

Equations (A2) and (A3) imply

$$\mathbf{P} = \frac{\hbar}{2\Delta_q}(\mathbf{A}^\dagger + \mathbf{A}), \tag{A29}$$

$$\mathbf{Q} = \frac{\hbar}{2i\Delta_p}(\mathbf{A}^\dagger - \mathbf{A}). \tag{A30}$$

Accordingly, we obtain the following from Eqs. (A24) and (A26):

$$\langle \mathbf{w},\mathbf{a}|\mathbf{P}|\mathbf{w},\mathbf{a}\rangle = \mathbf{w}, \tag{A31}$$

$$\langle \mathbf{w},\mathbf{a}|\mathbf{Q}|\mathbf{w},\mathbf{a}\rangle = \mathbf{a}, \tag{A32}$$

which shows that the state $|\mathbf{w},\mathbf{a}\rangle$ is centered at the point $(\mathbf{w},\mathbf{a})$ in phase space. From Eqs. (A2), (A3), (A24), (A26), and (A29)–(A32) and by using Eq. (A4), we get the following for the mean square deviations:

$$\langle \mathbf{w},\mathbf{a}|(\mathbf{P} - \mathbf{w}\mathbb{1})^2|\mathbf{w},\mathbf{a}\rangle = \left(\frac{\hbar}{2\Delta_q}\right)^2 = \Delta_p^2,$$

$$\langle \mathbf{w},\mathbf{a}|(\mathbf{Q} - \mathbf{a}\mathbb{1})^2|\mathbf{w},\mathbf{a}\rangle = \left(\frac{\hbar}{2\Delta_p}\right)^2 = \Delta_q^2,$$

i.e., all states $|\mathbf{w},\mathbf{a}\rangle$ saturate the Heisenberg inequalities independent of their position. In fact, by construction [see Eq. (A25)], these states are nothing else but the coherent state $|\mathbf{0},\mathbf{0}\rangle$ translated in phase space.

By using Eqs. (A22) and (A25), we can express the scalar product $\langle \mathbf{w}',\mathbf{a}'|\mathbf{w},\mathbf{a}\rangle$ as

$$\begin{aligned}\langle \mathbf{w}_1,\mathbf{a}_1|\mathbf{w}_2,\mathbf{a}_2\rangle &= \langle \mathbf{0},\mathbf{0}|T(\mathbf{a}_1,\mathbf{w}_1)^{-1}T(\mathbf{a}_2,\mathbf{w}_2)|\mathbf{0},\mathbf{0}\rangle \\ &= \langle \mathbf{0},\mathbf{0}|T(-\mathbf{a}_1,-\mathbf{w}_1)T(\mathbf{a}_2,\mathbf{w}_2)|\mathbf{0},\mathbf{0}\rangle.\end{aligned} \tag{A33}$$

In order to evaluate the right-hand side of the above expression, we first calculate the product of translation operators. With

$$\begin{aligned}&[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)] \\ &= \left(\frac{i}{\hbar}\right)^2[-\mathbf{w}_1\cdot\mathbf{Q} + \mathbf{a}_1\cdot\mathbf{P}, \mathbf{w}_2\cdot\mathbf{Q} - \mathbf{a}_2\cdot\mathbf{P}] \\ &= \frac{i}{\hbar}(\mathbf{w}_2\cdot\mathbf{a}_1 - \mathbf{w}_1\cdot\mathbf{a}_2)\mathbb{1},\end{aligned}$$

which directly follows from the definition Eq. (A18) and the commutation relations in Eq. (A1), we obtain the following from Eqs. (A17) and (A21):

$$\begin{aligned}&T(-\mathbf{a}_1,-\mathbf{w}_1)T(\mathbf{a}_2,\mathbf{w}_2) \\ &= e^{G(-\mathbf{a}_1,-\mathbf{w}_1)}e^{G(\mathbf{a}_2,\mathbf{w}_2)} \\ &= e^{G(-\mathbf{a}_1,-\mathbf{w}_1)+G(\mathbf{a}_2,\mathbf{w}_2)}e^{(1/2)[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)]} \\ &= T(\mathbf{a}_2-\mathbf{a}_1,\mathbf{w}_2-\mathbf{w}_1)e^{(1/2)[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)]} \\ &= T(\mathbf{a}_2-\mathbf{a}_1,\mathbf{w}_2-\mathbf{w}_1)e^{(i/2\hbar)(\mathbf{w}_2\cdot\mathbf{a}_1-\mathbf{w}_1\cdot\mathbf{a}_2)}.\end{aligned} \tag{A34}$$

Let us now calculate the matrix element $\langle \mathbf{0},\mathbf{0}|T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle$. According to Eqs. (A18), (A29), (A30), and (A24), we have

$$G(-\mathbf{a},-\mathbf{w}) = \frac{i}{\hbar}(\mathbf{w}\cdot\mathbf{Q} - \mathbf{a}\cdot\mathbf{P}) = \boldsymbol{\alpha}\cdot\mathbf{A}^\dagger - \boldsymbol{\alpha}^\star\cdot\mathbf{A}.$$

From Eq. (A21) and the commutation relations in Eq. (A5), we get

$$T(\mathbf{w},\mathbf{a}) = e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger - \boldsymbol{\alpha}^\star\cdot\mathbf{A}} = e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger}e^{-\boldsymbol{\alpha}^\star\cdot\mathbf{A}}e^{-\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}^\star/2}.$$

Thus, by using Eq. (A6) and inserting definition (A24), we find

$$\begin{aligned}\langle \mathbf{0},\mathbf{0}|T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle &= e^{-\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}^\star/2}\langle \mathbf{0},\mathbf{0}|e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger}e^{-\boldsymbol{\alpha}^\star\cdot\mathbf{A}}|\mathbf{0},\mathbf{0}\rangle \\ &= e^{-\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}^\star/2} = e^{-(1/2)(\mathbf{w}^2/(2\Delta p)^2+\mathbf{a}^2/(2\Delta q)^2)}.\end{aligned} \tag{A35}$$

Putting together Eqs. (A33)–(A35), we finally obtain

$$\begin{aligned}\langle \mathbf{w}_1,\mathbf{a}_1|\mathbf{w}_2,\mathbf{a}_2\rangle &= e^{-(1/2)((\mathbf{w}_2-\mathbf{w}_1)^2/(2\Delta p)^2+(\mathbf{a}_2-\mathbf{a}_1)^2/(2\Delta q)^2)} \\ &\times e^{(i/2\hbar)(\mathbf{w}_2\cdot\mathbf{a}_1-\mathbf{w}_1\cdot\mathbf{a}_2)}.\end{aligned} \tag{A36}$$

The states $|\mathbf{n}\rangle$ defined by Eq. (A15) form a complete orthonormal basis in the one-particle Hilbert space $\mathcal{H}$. The following closure relation:

$$\sum_{n_1,n_2,n_3} |n_1,n_2,n_3\rangle\langle n_1,n_2,n_3| = \mathbb{1}$$

allows us, in particular, to express $|\mathbf{w},\mathbf{a}\rangle$ as

$$|\mathbf{w},\mathbf{a}\rangle = \sum_{n_1,n_2,n_3} |n_1,n_2,n_3\rangle\langle n_1,n_2,n_3|\mathbf{w},\mathbf{a}\rangle.$$

The coefficients $\langle n_1,n_2,n_3|\mathbf{w},\mathbf{a}\rangle$ or $\langle n_1,n_2,n_3|\boldsymbol{\alpha}\rangle$ in the notation of Eq. (A27) can be directly obtained from Eqs. (A16) and (A15). We immediately get

$$\langle \mathbf{n}|\boldsymbol{\alpha}\rangle = \frac{1}{\sqrt{n_1!\,n_2!\,n_3!}}\langle \mathbf{0}|A_1^{n_1}A_2^{n_2}A_3^{n_3}|\boldsymbol{\alpha}\rangle = \frac{\alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}}{\sqrt{n_1!\,n_2!\,n_3!}}\langle \mathbf{0}|\boldsymbol{\alpha}\rangle,$$

where we have used Eq. (A26) in the last line. With the closure relation for the states $|\mathbf{n}\rangle$, we get

$$1 = \langle \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle = \sum_{n_1,n_2,n_3} \langle \boldsymbol{\alpha}|n_1,n_2,n_3\rangle\langle n_1,n_2,n_3|\boldsymbol{\alpha}\rangle$$
$$= \sum_{n_1,n_2,n_3} \frac{|\alpha_1|^{2n_1}|\alpha_2|^{2n_2}|\alpha_3|^{2n_3}}{n_1!\,n_2!\,n_3!}|\langle \mathbf{0}|\boldsymbol{\alpha}\rangle|^2.$$

From Eq. (A36), we obtain

$$\langle \mathbf{0}|\boldsymbol{\alpha}\rangle = e^{-|\boldsymbol{\alpha}|^2/2},$$

and thus,

$$\langle \mathbf{n}|\boldsymbol{\alpha}\rangle = \frac{\alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}}{\sqrt{n_1!\,n_2!\,n_3!}}e^{-|\boldsymbol{\alpha}|^2/2}. \tag{A37}$$

The coherent states satisfy the following generalized closure relation:

$$\frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}| = \mathbb{1}. \tag{A38}$$

In order to prove this, we start from Eqs. (A19) and (A20), which imply

$$T(\delta\mathbf{a},\delta\mathbf{w})^{-1}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|T(\delta\mathbf{a},\delta\mathbf{w})$$
$$= |\mathbf{w}+\delta\mathbf{w},\mathbf{a}+\delta\mathbf{a}\rangle\langle\mathbf{w}+\delta\mathbf{w},\mathbf{a}+\delta\mathbf{a}|,$$

and, thus, also

$$\int d^3\mathbf{w}\int d^3\mathbf{a}T(\delta\mathbf{a},\delta\mathbf{w})^{-1}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|T(\delta\mathbf{a},\delta\mathbf{w})$$
$$= \int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|. \tag{A39}$$

For infinitesimal $\delta\mathbf{a}$ and $\delta\mathbf{w}$, we have the following according to Eqs. (A17) and (A18):

$$T(\delta\mathbf{a},\delta\mathbf{w}) \simeq \mathbb{1} + \frac{i}{\hbar}(\delta\mathbf{w}\mathbf{Q} - \delta\mathbf{a}\mathbf{P}).$$

By inserting this expression into Eq. (A39), we see that, necessarily,

$$\left[\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|,\mathbf{P}\right] = 0,$$

$$\left[\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|,\mathbf{Q}\right] = 0.$$

Since all operators $X \in \mathcal{L}(\mathcal{H})$ can be written as functions of $\mathbf{P}$ and $\mathbf{Q}$, it follows that

$$\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}| = c\mathbb{1}, \quad c \in \mathbb{C}.$$

Equation (A38) is obtained for the choice $c=(2\pi\hbar)^3$. This can be seen by calculating the matrix elements $\langle\mathbf{0},\mathbf{0}|\cdots|\mathbf{0},\mathbf{0}\rangle$. In fact, adopting the normalization $\langle\mathbf{0},\mathbf{0}|\mathbf{0},\mathbf{0}\rangle=1$, we get

$$\frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}\langle\mathbf{0},\mathbf{0}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|\mathbf{0},\mathbf{0}\rangle$$
$$= \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}e^{-((\mathbf{w})^2/(2\Delta p)^2+(\mathbf{a})^2/(2\Delta q)^2)}$$
$$= \langle\mathbf{0},\mathbf{0}|\mathbf{0},\mathbf{0}\rangle = 1,$$

where, in the second line, we used expression (A36) for the evaluation of the scalar product $\langle\mathbf{0},\mathbf{0}|\mathbf{w},\mathbf{a}\rangle$.

Due to the analytical properties of the coherent states with respect to the parameters $\mathbf{w},\mathbf{a}$ [or $\boldsymbol{\alpha}$, see Eq. (A24)], all matrix elements $\langle\boldsymbol{\alpha}|O|\boldsymbol{\alpha}'\rangle$ of a one-particle operator O can be reconstructed from its "diagonal" matrix elements $\langle\boldsymbol{\alpha}|O|\boldsymbol{\alpha}\rangle$, where the states $|\boldsymbol{\alpha}\rangle$ are written in the shorthand notation (A27). In order to prove this quite surprising property, which is sometimes referred to as the "diagonal representation," we have to show that

$$\langle\boldsymbol{\alpha}|X|\boldsymbol{\alpha}\rangle = \langle\boldsymbol{\alpha}|Y|\boldsymbol{\alpha}\rangle, \quad \forall\ \boldsymbol{\alpha}, \tag{A40}$$

implies

$$Z \equiv X - Y = 0.$$

We start from the fact that the eigenstates of the self-adjoint operator $\mathbf{A}^\dagger\mathbf{A}$ form a complete orthonormal basis. From Eq. (A16), we get

$$\mathbf{A}^\dagger\cdot\mathbf{A}|\mathbf{n}\rangle = n|\mathbf{n}\rangle, \quad \mathbf{n} = (n_1,n_2,n_3),$$
$$\text{with } n_i = 0,1,2,\ldots,\ i = 1,2,3.$$

The completeness of the states $|\mathbf{n}\rangle$ implies

$$\sum_{\mathbf{n}}|\mathbf{n}\rangle\langle\mathbf{n}| = \mathbb{1}.$$

Thus, Eq. (A40) can be rewritten in the following form:

$$0 \equiv \langle\boldsymbol{\alpha}|Z|\boldsymbol{\alpha}\rangle = \sum_{\mathbf{n}}\sum_{\mathbf{m}}\langle\boldsymbol{\alpha}|\mathbf{n}\rangle\langle\mathbf{n}|Z|\mathbf{m}\rangle\langle\mathbf{m}|\boldsymbol{\alpha}\rangle. \tag{A41}$$

By inserting Eq. (A37), which is written in the following shorthand notation:

$$\langle\boldsymbol{\alpha}|\mathbf{n}\rangle = \frac{\boldsymbol{\alpha}^{\star\mathbf{n}}}{\sqrt{\mathbf{n}!}}e^{-|\boldsymbol{\alpha}|^2/2},$$

where $\mathbf{n}!\equiv n_1!n_2!n_3!$ and $\boldsymbol{\alpha}^{\mathbf{n}}\equiv\alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}$, into Eq. (A41), we obtain the following condition:

$$\sum_{\mathbf{n}}\sum_{\mathbf{m}}\frac{\boldsymbol{\alpha}^{\star\mathbf{n}}\boldsymbol{\alpha}^{\mathbf{m}}}{\sqrt{\mathbf{n}!\,\mathbf{m}!}}\langle\mathbf{n}|Z|\mathbf{m}\rangle \equiv 0,$$

which implies

$$\langle\mathbf{n}|Z|\mathbf{m}\rangle = 0, \quad \forall\ \mathbf{n},\mathbf{m},$$

and thus, $Z=0$. This important property implies, in particular, that the operator O can be written in the following form:

$$O = \int_{\mathbb{R}^6} d^6z\, o(z)\, |z\rangle\langle z|$$

$$= \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} d^3\mathbf{w} \int_{\mathbb{R}^3} d^3\mathbf{a}\, o(\mathbf{w},\mathbf{a})\, |\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|, \tag{A42}$$

which is sometimes referred to as the diagonal representation. From Eq. (A42) and the definition of the overlap function $g(z,z')$ given by Eq. (18), we find that the function $o(z)$ and the diagonal elements $\langle z|O|z\rangle$ are related by the following integral equation:

$$\langle z|O|z\rangle = \int_{\mathbb{R}^6} d^6z'\, o(z')g(z,z').$$

APPENDIX B: SOLUTION OF THE INTEGRAL EQUATION (21)

With Eq. (17), the integral Eq. (21) becomes

$$p(z,s) = \int_{\mathbb{R}^6} d^6z'\, \rho(z',s)g(z,z'). \tag{B1}$$

This equation can be solved by using the matrix inversion method proposed in Ref. 24. According to Eq. (18), the kernel depends only on the difference $z-z'$, i.e., we may write

$$g(z,z') \equiv h(z-z') = h_1(\mathbf{q}-\mathbf{q}')h_2(\mathbf{p}-\mathbf{p}'), \tag{B2}$$

where

$$h_1(\mathbf{q}-\mathbf{q}') = e^{-[(\mathbf{q}-\mathbf{q}')/2\Delta]^2},$$

$$h_2(\mathbf{p}-\mathbf{p}') = e^{-[(\mathbf{p}-\mathbf{p}')\Delta/\hbar]^2}.$$

We start from the Taylor expansion of $\rho(z',s)$ at z,

$$\rho(z',s) = \sum a_n\rho^{(n)}(z), \tag{B3}$$

where

$$\rho^{(n)}(z,s) \equiv \left(\frac{\partial}{\partial z'}\right)^n \rho(z',s)\bigg|_{z'=z}$$

and

$$a_n = \frac{1}{n!}\int_{\mathbb{R}^6} d^6z'(z')^n h(z),$$

where $(z')^n$ denotes the following six-dimensional vector:

$$(z')^n \equiv \left[\left(\frac{\Delta_q}{\pi\hbar}p_1'\right)^n, \left(\frac{\Delta_q}{\pi\hbar}p_2'\right)^n, \left(\frac{\Delta_q}{\pi\hbar}p_3'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_1'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_2'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_3'\right)^n\right].$$

The symmetry of the function $h(z)$ defined in Eq. (B2) with respect to the origin implies

$$a_{2n+1} = 0, \quad n = 0,1,\ldots. \tag{B4}$$

By inserting Eq. (B3) into Eq. (B1), we get

$$p(z,s) = \sum_{n=0}^{\infty} a_n\rho^{(n)}(z,s).$$

By taking the derivatives of the above equation:

$$p^{(1)}(z,s) = \sum_{n=0}^{\infty} a_n\rho^{(n+1)}(z,s),$$

$$p^{(2)}(z,s) = \sum_{n=0}^{\infty} a_n\rho^{(n+2)}(z,s),$$

$$\cdots,$$

and by assuming that for some given integer m we have

$$p^{(j)}(z,s) \approx 0, \quad j > m, \tag{B5}$$

we obtain the following linear equation system:

$$\begin{pmatrix} p^{(0)}(z,s) \\ p^{(1)}(z,s) \\ \vdots \\ p^{(m)}(z,s) \end{pmatrix} = A \begin{pmatrix} \rho^{(0)}(z,s) \\ \rho^{(1)}(z,s) \\ \vdots \\ \rho^{(m)}(z,s) \end{pmatrix}, \tag{B6}$$

where

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_m \\ 0 & a_0 & a_1 & \cdots & a_{m-1} \\ & & \ddots & & \\ 0 & 0 & \cdots & & a_0 \end{pmatrix}.$$

The tridiagonal matrix A can be easily inverted. We have

$$B \equiv A^{-1} = \begin{pmatrix} b_0 & b_1 & b_2 & \cdots & b_m \\ 0 & b_0 & b_1 & \cdots & b_{m-1} \\ & & \ddots & & \\ 0 & 0 & \cdots & & b_0 \end{pmatrix},$$

where

$$\sum_{i=0}^{n} a_i b_{n-i} = \delta_{0n}, \quad n = 0,1,\ldots,m. \tag{B7}$$

From Eqs. (B4) and (B7), we get

$$b_{2n+1} = 0, \quad n = 0,1,\ldots,$$

and for the first nonvanishing b coefficients:

$$b_0 = \frac{1}{a_0}, \quad b_2 = -\frac{a_2}{a_0^2}, \quad b_4 = \frac{1}{a_0^2}\left(\frac{a_2^2}{a_0} - a_4\right),$$

$$b_6 = -\frac{1}{a_0^2}\left(\frac{a_2^3}{a_0^2} - 2\frac{a_2a_4}{a_0} + a_6\right),$$

$$\cdots.$$

Clearly, the solution of Eq. (B6):

$$\begin{pmatrix} \rho^{(0)}(z,s) \\ \rho^{(1)}(z,s) \\ \vdots \\ \rho^{(m)}(z,s) \end{pmatrix} = B \begin{pmatrix} p^{(0)}(z,s) \\ p^{(1)}(z,s) \\ \vdots \\ p^{(m)}(z,s) \end{pmatrix} \tag{B8}$$

satisfies condition (29) if condition (B5) is satisfied and if $|p^{(i)}(z,s)|<\infty$, $i=1,2,\ldots,m$. The validity of additional condition (31), which finally leads to the conventional form of the drift term and the field term in the semi-classical Boltzmann equation, requires that we can choose the parameter Δ such that $m=2$ in Eq. (B5). Thus, both conditions (29) and (31) are satisfied as long as, on the scale of the parameters Δ_q and Δ_p, the expectation values $p^{(0)}(z,s)$ depend only weakly on the position $\mathbf{p},\mathbf{q}$ in phase space.

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[17] Strictly speaking, the positivity of the *coarse-grained* one-particle density matrix $\bar{D}_1$ is not always guaranteed, i.e., for some vectors $|x\rangle\in\mathcal{H}$, the expectation value $\langle x|\bar{D}_1|x\rangle$ may be slightly negative. This deviation from the von Neumann properties of a density matrix, which is unavoidable if one considers the evolution of the system on the true time scale, scales with the strength of H_{int} and thus remains negligibly small. In the following, we will assume the positivity of the matrix elements $\langle\mathbf{u}|\bar{D}_1|\mathbf{u}\rangle$, where $|\mathbf{u}\rangle$ denotes a coherent state including the spin variable (for a detailed discussion, see Ref. 16).

[18] In order to simplify the notation, the kinetic-energy operator and the potential operator will be denoted V,T instead of $\hat{V},\hat{T}$ in the following. The hats in the functions $\hat{V}(\mathbf{k})$ are used to denote the Fourier transforms.

[19] The presently requested smooth behavior of the function $\rho(\mathbf{p},\mathbf{q},s)$ must be seen as a supplementary condition for the statistical state of the considered system. We remind the reader that, presently, we are investigating the conditions for which the system evolution can be described by the semi-classical Boltzmann equation. Clearly, we cannot expect or pretend that this covers the whole range of experiments in solid-state physics. Nevertheless, the large success of this type of approach in solid-state physics indicates that many experimental situations can be described by one-particle density matrices, where the functions $\rho(\mathbf{p},\mathbf{q},s)$ satisfy the conditions Eqs. (29) and (31).

[20] Note that the density matrix D_1 is positive. This holds also to a good approximation for the coarse-grained density matrix $\bar{D}_1$ (see also Ref. 17), i.e., we may safely assume that $p(\mathbf{u})=\langle\mathbf{u}|\bar{D}_1|\mathbf{u}\rangle\geq 0$. We also note that the $p(\mathbf{u})$ values depend on the chosen Δ parameter. This suggests that, if necessary, the positivity may also be reached by a judicious choice of Δ.

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