

Wigner transport models of the electron-phonon kinetics in quantum wiresM. Nedjalkov,¹ D. Vasileska,² D. K. Ferry,² C. Jacoboni,³ C. Ringhofer,⁴ I. Dimov,⁵ and V. Palankovski¹¹*AMADEA Group, IµE, TU-Vienna, Gusshausstrasse 27-29/E360 A-1040 Vienna, Austria*²*Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85287-1804, USA*³*University of Modena and Reggio Emilia, Via Campi 213/A, I-41100 Modena, Italy*⁴*Department of Mathematics, Arizona State University, Tempe, Arizona 85287-1804, USA*⁵*Institute for Parallel Processing, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria**and ACET Centre, University of Reading, Whiteknights P.O. Box 217, Reading RG6 6AH, United Kingdom*

(Received 17 April 2006; published 12 July 2006)

Two quantum-kinetic models of ultrafast electron transport in quantum wires are derived from the generalized electron-phonon Wigner equation. The various assumptions and approximations allowing one to find closed equations for the reduced electron Wigner function are discussed with an emphasis on their physical relevance. The models correspond to the Levinson and Barker-Ferry equations, now generalized to account for a space-dependent evolution. They are applied to study the quantum effects in the dynamics of an initial packet of highly nonequilibrium carriers, locally generated in the wire. The properties of the two model equations are compared and analyzed.

DOI: [10.1103/PhysRevB.74.035311](https://doi.org/10.1103/PhysRevB.74.035311)

PACS number(s): 73.23.-b, 02.50.Fz, 02.60.Cb, 02.70.Ss

I. INTRODUCTION

The early-time dynamics of highly nonequilibrium confined carriers incorporates a variety of phenomena, which, reflecting the uncertainty relations, are beyond the Boltzmann-like picture of the transport process. An instantaneous scattering process occurring between electron states with well-defined energy no longer provides an adequate description: Effects of time-dependent collisional broadening (CB) and retardation of phonon replicas have been investigated theoretically and experimentally in homogeneous semiconductors.¹⁻⁸ These effects are related to the lack of energy conservation and the memory character of the electron-phonon dynamics, and are due to the finite duration of the interaction process. The effect of the action of the electric field during the process of collision—the intracollisional field effect⁹⁻¹⁴ (ICFE)—has attracted scientific attention for quite some time. It has been shown that the intracollisional field effect is not important in stationary high-field transport in semiconductors when single-valley transport is considered.¹⁵⁻¹⁷ Rather, the effect must be sought in the time domain of the early-time evolution, which precedes the formation of the classical energy-conserving δ function.^{18,19}

A natural representation in spatially homogeneous systems is provided by wave vector space, which reflects momentum conservation. Kinetic model equations accounting for these effects were developed in the framework of Green's function²⁰⁻²² or density matrix formalisms.^{1,10,23,24} Explicitly or implicitly these approaches give rise to the Levinson²³ and/or Barker-Ferry¹⁰ equations. Indeed, a general model for photoexcited semiconductors is the set of semiconductor Bloch equations for the electron, hole, and phonon distributions and the interband polarization. Phenomena due to carrier-light, carrier-carrier, and carrier-phonon interactions are accounted for in a comprehensive way.⁸ The case of a single-band model, in the low-density regime, focuses on the

carrier-phonon interaction. In this case the polarization can be eliminated, giving rise to a generation rate, which furthermore is approximated by an initial condition. A set of equations is obtained for the electron and phonon distributions and the phonon-assisted density matrix.¹ Under the assumption of equilibrium phonons the set gives rise to the Barker-Ferry equation.²⁵ The latter can be considered as a generalization of the Levinson equation, which accounts for the finite electron lifetime due to the interaction with the phonons.

Confined systems are characterized by small spatial scales where another basic assumption of classical transport—this for a scattering process occurring at a well-defined position—loses its validity. In such systems the scattering is no longer local in space due to the finite duration of the carrier-phonon interaction. The introduction of a spatial coordinate allows one to account for inhomogeneities which can be due to the structure of the sample or due to the confinement of the initial condition. In such cases a convenient description of the transport is given by the Wigner-function formalism. It retains most of the basic classical notions, in particular the concepts for phase space and a distribution function. Averaged values of the physical quantities in Boltzmann and Wigner pictures are expressed with the same functionals of the corresponding distribution functions. Another advantage of the Wigner picture is the opportunity to utilize Newton's trajectories^{26,27} along with the properties of the Liouville theorem. This allows one to interpret the entire quantum evolution, and in particular the interaction with the Wigner potential, in terms of particles.²⁸ Both classical and quantum particles evolve over segments of Newton's trajectories. However, because of the nonlocal nature of the scattering, evolution trajectories inherent to Boltzmann particles are generalized by Wigner paths.²⁹ The latter in principle lead to a different spatial distribution of the system.¹⁷ In general, in contrast to a classical distribution, the Wigner function can have negative values which manifests the uncertainty relation and thus the quantum character of the evolution.³⁰

Physical systems which combine short spatial and time scales recently have become a field of active research interest. An equation, which under homogeneous conditions reduces to the Levinson equation, has been derived within a Green's function approach by using the generalized Kadanoff-Baym ansatz.³¹ Wigner equation models for nanometer and femtosecond transport regimes have been recently proposed in Refs. 32 and 33. It has been shown that the case of a constant electric field gives rise to a Levinson-type equation which accounts for the spatial dimensions.³² The complex case of arbitrary band structure, general electric field and inhomogeneous impurity distribution has been resolved by Krieger *et al.*³³ The semiconductor Bloch equations have been generalized for spatially inhomogeneous excitations by using a density matrix approach.¹⁹ The Wigner counterparts of the equations are then obtained by using a Fourier transform for two- and single-band models. The latter gives rise to an inhomogeneous generalization of the Levinson equation. The models have been compared for the case of spatiotemporal evolution of a local electron distribution, optically generated in a quantum wire. The comparison shows that the typical quantum-kinetic features of the carrier-phonon interaction in the single-band model and the physically comprehensive two-band model are essentially the same. From here it can be concluded that the Levinson and Barker-Ferry models provide a relevant description of these features.

Quantum-kinetic effects in the evolution of carriers, confined in quantum wires, have been investigated in the framework of the Barker-Ferry model derived with the help of a projection technique.³⁴ Actually the Levinson model is derived and a factor accounting for the finite electron lifetime has been introduced by heuristic considerations.³⁵ Memory effects have been neglected by taking the Markovian limit of the equation. This approach leads to a Boltzmann-like equation where the classical δ function is replaced by a Lorentzian. The equation has been solved by a modification of the classical ensemble Monte Carlo method. The solutions, obtained at different evolution times well demonstrate stationary ICFE and CB effects. However, we note that at larger evolution times the approach based on stationary broadening of the energy conservation can lead to unphysical solutions. The reason is in the long-reaching wings of the Lorentzian which can cause artificial heating of the carrier system.^{12,36–38}

In this paper we utilize the Wigner formalism to derive the Levinson and Barker-Ferry equations for the carrier-phonon kinetics in a quantum wire. First we obtain the generalized Wigner function³⁹ (GWF) of the carrier-phonon system in the wire. Of interest is the reduced, or electron, Wigner function obtained from the diagonal with respect to the phonon basis GWF elements. The latter are linked by the corresponding equation of motion to first off-diagonal (FOD) elements which differ by adding or subtracting a single phonon in a given mode \mathbf{q} in the left or right basis. The FOD elements are linked to second off-diagonal elements (SOD), etc., which gives rise to an infinite hierarchy of equations coupled by the phonon degrees of freedom. A closure is obtained by consecutive steps of assumptions and approximations. Frequently applied will be the random phase approxi-

mation which is used to neglect the rapidly oscillating “in-time” terms. A Markov approximation will be used to derive the factor accounting for the finite carrier lifetime of the Barker-Ferry model. The trace operation is applied at the very end, after the truncation of the hierarchy, which is another peculiarity of our approach.

The physical relevance of the two models as well as the heuristic aspects of the formal steps of finding closed equations for the electron function are discussed in the second part of the paper. In particular the requirements ensuring an equilibrium phonon system are analyzed beyond the Bloch assumption.

Finally we present simulation results for the evolution of an initial electron distribution in a rectangular quantum wire. Extreme conditions of very low temperature are chosen. In this case the evolution of classical electrons is very transparent as they can only lose energy to the phonons. Moreover, quantum electrons can be considered in the ground state in the plane normal to the wire. The classical evolution provides a background which is used to outline the quantum effects introduced by the models explored. We analyzed the behavior of the physical observables corresponding to the first moments of the Wigner function: the concentration, the wave vector distribution, and the energy density. The simulation results are obtained by a backward Monte Carlo method. This method allows a pointwise evaluation of the Wigner function and the corresponding moments to a desired precision.

II. GENERALIZED WIGNER EQUATION

A. Formulation of the transport problem

We consider a low-density system of electrons evolving in a quantum wire and interacting with the lattice vibrations. The description of the system is provided by both electron and phonon degrees of freedom. We first generalize the Wigner function and the Wigner equation for the coupled electron-phonon system in the wire. The Hamiltonian of the system,

$$H = H_0 + V + H_p + H_{e-p} = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}} + V(\mathbf{r}) + \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \hbar \omega_{\mathbf{q}} + i\hbar \sum_{\mathbf{q}} F(\mathbf{q})(b_{\mathbf{q}} e^{i\mathbf{q}\cdot\hat{\mathbf{r}}} - b_{\mathbf{q}}^\dagger e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}), \quad (1)$$

is given by the free electron part H_0 , the wire potential $V(\mathbf{r})$ the free-phonon Hamiltonian H_p , and the electron-phonon interaction H_{e-p} . Here $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$ are the creation and annihilation operators for the phonon mode \mathbf{q} , $\hbar \omega_{\mathbf{q}}$ is the energy of the mode, and $F(\mathbf{q})$ is the electron-phonon coupling element, which depends on the type of phonon scattering analyzed. The state of the phonon subsystem is represented by the set $\{n_{\mathbf{q}}\} = \{n_{\mathbf{q}_1}, n_{\mathbf{q}_2}, \dots\}$ where $n_{\mathbf{q}}$ is the occupation number of the phonons in mode \mathbf{q} . Then the representation is given by the vectors $|\{n_{\mathbf{q}}\}, \mathbf{r}\rangle = |\{n_{\mathbf{q}}\}\rangle |\mathbf{r}\rangle$. A homogeneous electric field $E(t)$ can be applied along the z direction of the wire; the carriers are assumed confined in the normal plane. For a transparent presentation we assume a stationary electric field and a

ground state Ψ in the normal to the wire axis:

$$H_0 + V(\mathbf{r}) = H_{\perp} + H_z = H_{0\perp} + V_{\perp} + H_{0z} + V(z),$$

where $H_{\perp}\Psi = E_{\perp}\Psi$, $V(z) = -eEz$ and $|\mathbf{r}\rangle = |\mathbf{r}_{\perp}\rangle|z\rangle$. The generalization for time-dependent fields and a set of subbands is straightforward.

The electron-phonon Wigner function is defined by the Fourier transform of the density operator $\hat{\rho}_t$:

$$f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t) = \frac{1}{2\pi\hbar} \int dz' \int d\mathbf{r}_{\perp} e^{-ip_z z' / \hbar} \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \hat{\rho}_t | \mathbf{r}_{\perp} \right\rangle \left\langle \mathbf{r}_{\perp} | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle.$$

Separating of the transport in the normal plane and the z direction we have $\hat{\rho}_t = |\Psi\rangle\langle\Psi| \hat{\rho}_{tz}$:

$$\langle \mathbf{r}, \{n_{\mathbf{q}}\} | \hat{\rho}_t | \{n'_{\mathbf{q}}\}, \mathbf{r}' \rangle = \Psi^*(\mathbf{r}_{\perp}) \Psi(\mathbf{r}_{\perp}) \rho(z, z', \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t).$$

Finally the requirement for normalization of Ψ leads to

$$f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t) = \frac{1}{2\pi\hbar} \int dz' e^{-ip_z z' / \hbar} \rho \left(z + \frac{z'}{2}, z - \frac{z'}{2}, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t \right).$$

B. Derivation of the generalized Wigner equation

The equation of motion of f_w is obtained from the von Neumann equation for the density matrix:

$$\begin{aligned} & \frac{\partial f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t)}{\partial t} \\ &= \int \frac{dz'}{i2\pi\hbar^2} \int d\mathbf{r}_{\perp} e^{-ip_z z' / \hbar} \\ & \times \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \langle \mathbf{r}_{\perp} | [H, \hat{\rho}_t] | \mathbf{r}_{\perp} \rangle | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle. \end{aligned}$$

For convenience the right-hand side of this equation is denoted by $\text{WT}(H)$. By following the steps used to introduce the common GWF,³⁹⁻⁴¹ we evaluate $\text{WT}(H)$ for each term of the wire Hamiltonian (1). $\text{WT}(H_{\perp})$ gives zero for the ground state in the normal direction. $\text{WT}(H_{0z})$ and $\text{WT}(-eEz)$ are readily calculated by using integration by parts:

$$\text{WT}(H_{0z}) = -\frac{p_z}{m} \frac{\partial f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t)}{\partial z},$$

$$\text{WT}(-eEz) = -eE \frac{\partial f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t)}{\partial p_z}.$$

The free phonon term gives rise to

$$\text{WT}(H_p) = \frac{1}{i\hbar} [\epsilon(\{n_{\mathbf{q}}\}) - \epsilon(\{n'_{\mathbf{q}}\}) f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t)],$$

where $\epsilon(\{n_{\mathbf{q}}\}) = \sum_{\mathbf{q}} n_{\mathbf{q}} \hbar \omega_{\mathbf{q}}$. $\text{WT}(H_{e-p})$ consists of four contributions arising from the commutator of the density operator

with the phonon creation and annihilation operators. They are evaluated with the help of the decomposition of the unity:

$$1 = \int dz'' |z''\rangle\langle z''| \int d\mathbf{r}''_{\perp} |\mathbf{r}''_{\perp}\rangle\langle \mathbf{r}''_{\perp}|.$$

As \mathbf{q} has been already used in the notation of the phonon basis, the phonon mode in H_{e-p} , (1) is replaced by \mathbf{q}' .

The first contribution of $\text{WT}(H_{e-p})$ is estimated as the sum over \mathbf{q}' of term as the following:

$$\begin{aligned} \text{I} &= \frac{1}{2\pi\hbar} \int d\mathbf{r}_{\perp} \int dz' \int d\mathbf{r}'' e^{-ip_z z' / \hbar} \\ & \times \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \langle \mathbf{r}_{\perp} | b_{\mathbf{q}'} e^{i\mathbf{q}' \cdot \mathbf{r}''} | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{\rho}_t | \mathbf{r}_{\perp} \rangle | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle \\ &= \sqrt{n_{\mathbf{q}'} + 1} \int d\mathbf{r}_{\perp} e^{i\mathbf{q}'_{\perp} \cdot \mathbf{r}_{\perp}} |\Psi(\mathbf{r}_{\perp})|^2 \int dz' e^{-ip_z z' / \hbar} e^{i\mathbf{q}'_{\perp} (z+z')/2} \\ & \times \left\langle z + \frac{z'}{2}, \{n_1, \dots, n_{\mathbf{q}'} + 1, \dots\} | \hat{\rho}_{tz} | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle \\ &= \sqrt{n_{\mathbf{q}'} + 1} G(\mathbf{q}'_{\perp}) e^{i\mathbf{q}'_{\perp} z} f_w \left(z, p_z - \frac{\hbar \mathbf{q}'_{\perp}}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n'_{\mathbf{q}}\}, t \right), \end{aligned}$$

where G denotes the Fourier transform of $|\Psi(\mathbf{r}_{\perp})|^2$. We used the normalization of the position basis $\langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')$ and the fact that $b_{\mathbf{q}}$ becomes a creation operator when operating to the left. The shorthand notations $\{n_{\mathbf{q}}\}_{\mathbf{q}'}^{\pm} = \{n_1, \dots, n_{\mathbf{q}'} \pm 1, \dots\}$ are introduced. In this way $\{n_{\mathbf{q}}\}_{\mathbf{q}'}^{\pm}$ ($\{n_{\mathbf{q}}\}_{\mathbf{q}'}^{\mp}$) are states of the phonon subsystem, obtained from $\{n_{\mathbf{q}}\}$ by increasing (decreasing) the number of phonons in the mode \mathbf{q}' by unity. In a similar way,

$$\begin{aligned} \text{II} &= -\frac{1}{2\pi\hbar} \int d\mathbf{r}_{\perp} \int dz' e^{-ip_z z' / \hbar} \\ & \times \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \langle \mathbf{r}_{\perp} | b_{\mathbf{q}'}^{\dagger} e^{-i\mathbf{q}' \cdot \mathbf{r}''} \hat{\rho}_t | \mathbf{r}_{\perp} \rangle | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle \\ &= -\sqrt{n_{\mathbf{q}'}} G^*(\mathbf{q}'_{\perp}) e^{-i\mathbf{q}'_{\perp} z} f_w \left(z, p_z + \frac{\hbar \mathbf{q}'_{\perp}}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, \{n'_{\mathbf{q}}\}, t \right). \end{aligned}$$

We note that half of the z component of the phonon mode is added to the electron momentum p_z . The sign of q'_z is opposite to the sign of the argument in the corresponding exponent. The phonon annihilation and creation operators of the next two contributions change the right phonon basis:

$$\begin{aligned} \text{III} &= -\frac{1}{2\pi\hbar} \int d\mathbf{r}_{\perp} \int dz' e^{-ip_z z' / \hbar} \\ & \times \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \langle \mathbf{r}_{\perp} | \hat{\rho}_t b_{\mathbf{q}'} e^{i\mathbf{q}' \cdot \mathbf{r}''} | \mathbf{r}_{\perp} \rangle | \{n'_{\mathbf{q}}\}, z - \frac{z'}{2} \right\rangle \\ &= -\sqrt{n'_{\mathbf{q}'}} G(\mathbf{q}'_{\perp}) e^{i\mathbf{q}'_{\perp} z} f_w \left(z, p_z + \frac{\hbar \mathbf{q}'_{\perp}}{2}, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}_{\mathbf{q}'}^-, t \right). \end{aligned}$$

Here the signs of the phonon mode added to p_z and in the

exponent in front of f_w are the same. Finally the fourth term is

$$\begin{aligned} \text{IV} &= \frac{1}{2\pi\hbar} \int d\mathbf{r}_\perp \int dz' \int d\mathbf{r}'' e^{-ip_z z'/\hbar} \\ &\quad \times \left\langle z + \frac{z'}{2}, \{n_{\mathbf{q}}\} | \langle \mathbf{r}_\perp | \hat{\rho}_t b_{\mathbf{q}}^\dagger e^{-i\mathbf{q}' \cdot \mathbf{r}''} | \mathbf{r}_\perp \rangle | \{n_{\mathbf{q}}'\}, z - \frac{z'}{2} \right\rangle \\ &= \sqrt{n_{\mathbf{q}'} + 1} G^*(\mathbf{q}'_\perp) e^{-iq'_z z' f_w} \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}'\}^+, t \right). \end{aligned}$$

By collecting all contributions we obtain the equation of motion of the GWF in the wire:

$$\begin{aligned} &\left(\frac{\partial}{\partial t} + \frac{p_z}{m} \nabla_z + eE \nabla_{p_z} \right) f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}'\}, t) \\ &= \frac{1}{i\hbar} [\epsilon(\{n_{\mathbf{q}}\}) - \epsilon(\{n_{\mathbf{q}}'\})] f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}'\}, t) \\ &+ \sum_{\mathbf{q}'} F(\mathbf{q}') \left\{ G(\mathbf{q}'_\perp) e^{iq'_z z} \sqrt{n_{\mathbf{q}'} + 1} \right. \\ &\quad \times f_w \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}'\} \right) \\ &\quad - G^*(\mathbf{q}'_\perp) e^{-iq'_z z} \sqrt{n_{\mathbf{q}'}} f_w \left(z, p_z + \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, \{n_{\mathbf{q}}'\}, t \right) \\ &\quad - G(\mathbf{q}'_\perp) e^{iq'_z z} \sqrt{n_{\mathbf{q}'}} f_w \left(z, p_z + \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}'\}_{\mathbf{q}'}^-, t \right) \\ &\quad \left. + G^*(\mathbf{q}'_\perp) e^{-iq'_z z} \sqrt{n_{\mathbf{q}'}} + 1 f_w \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}'\}_{\mathbf{q}'}^+, t \right) \right\}. \end{aligned} \quad (2)$$

The generalized Wigner equation couples an element $f_w(\dots, \{n\}, \{m\}, t)$ to four neighboring elements with one phonon added or subtracted in the left or right basis for the particular mode \mathbf{q}' of the sum. For all modes \mathbf{q} the number of phonons $n_{\mathbf{q}}$ can be any integer between 0 and infinity and the sum over \mathbf{q}' couples all modes.

The equation can not be solved without relevant criteria aiming to neglect most of the GWF elements. A natural hierarchy in the set of elements is introduced by the fact that the pertinent physical information about the electron subsystem is provided by the main diagonal of Eq. (2): the reduced Wigner function is defined by the trace

$$f_w(z, p_z, t) = \sum_{\{n_{\mathbf{q}}\}} f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t) \quad (3)$$

of the generalized Wigner function $f_w(\dots, \{n\}, \{n\}, t)$, diagonal with respect to the phonon coordinates.

In this respect appropriate hypotheses are the assumptions for an initially decoupled electron-phonon system, weak interaction, and equilibrium phonons. A useful tool for neglecting terms is the random phase approximation⁴² (RPA). In a sum of the type $\sum_{\mathbf{q}, \mathbf{q}'} \exp\{i[f(\mathbf{q}) - f(\mathbf{q}')]t\}$ this approximation essentially retains the terms $\mathbf{q} = \mathbf{q}'$ and neglects the rapidly oscillating terms which more or less average to zero. Con-

sider the imaginary term determined by the difference of the energies of the left and right phonon states. As seen from the integral form of the equation (Appendix A), this term is related to the frequency of the oscillations in time of the GWF. This frequency will be the main argument in the process of comparison of the consecutive terms in the hierarchy.

According to these consideration we must begin with the equation for the diagonal elements.

C. Equation for the diagonal elements

By denoting $F'_G = F(\mathbf{q}')G(\mathbf{q}'_\perp)$ the equation reads

$$\begin{aligned} &\left(\frac{\partial}{\partial t} + \frac{p_z}{m} \nabla_z + eE \nabla_{p_z} \right) f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t) \\ &= \sum_{\mathbf{q}'} \left\{ F'_G e^{iq'_z z} \sqrt{n_{\mathbf{q}'} + 1} f_w \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t \right) \right. \\ &\quad - F'^*_G e^{-iq'_z z} \sqrt{n_{\mathbf{q}'}} f_w \left(z, p_z + \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, \{n_{\mathbf{q}}\}, t \right) \\ &\quad - F'_G e^{iq'_z z} \sqrt{n_{\mathbf{q}'}} f_w \left(z, p_z + \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, t \right) \\ &\quad \left. + F'^*_G e^{-iq'_z z} \sqrt{n_{\mathbf{q}'}} + 1 f_w \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, t \right) \right\}. \end{aligned} \quad (4)$$

The equation requires an initial condition, corresponding to a noninteracting system, where the phonons are assumed in equilibrium.

We note the lack of the imaginary term, which means that diagonal elements do not show the oscillatory behavior typical for the off-diagonal elements. A diagonal element is linked to FOD elements, which are diagonal in all modes but the current mode \mathbf{q}' of the summation. In this mode the four neighbors of $n_{\mathbf{q}'}, n_{\mathbf{q}'}$ —namely $n_{\mathbf{q}'} \pm 1, n_{\mathbf{q}'}$ and $n_{\mathbf{q}'}, n_{\mathbf{q}' \pm 1}$ —are concerned. We need to consider only the FOD elements contained in the first two terms on the right: From the definition of f_w and (4) it follows that the third and fourth terms are conjugated to the second and first terms, respectively.

In general the equations for $f_{FOD}^\pm = f_w(\cdot, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^\pm, \{n_{\mathbf{q}}\}, \cdot)$ introduce SOD elements. We pursue the idea to truncate the hierarchy by neglecting the second- and higher-order off-diagonal elements. It is necessary to write explicitly all algebraic details in order to recognize the few terms which must remain in the right-hand sides of the equations.

III. TRUNCATION AT THE FOD LEVEL

A. Equations for the FOD elements

In what follows we use the abbreviation $F''_G = F_G(\mathbf{q}'')$. The equations of motion for f_{FOD}^+ and f_{FOD}^- can be unified as follows:

$$\begin{aligned}
& \left(\frac{\partial}{\partial t} + \frac{p_z \mp \frac{\hbar q'_z}{2}}{m} \nabla_z + eE \nabla_{p_z} \pm i\omega_{\mathbf{q}'} \right) f_w \left(z, p_z \mp \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t \right) \\
& = \sum_{\mathbf{q}''} \left\{ F_G'' e^{iq''_z z} \sqrt{n_{\mathbf{q}''}} + 1 f_w \left(z, p_z \mp \frac{\hbar(q'_z \pm q''_z)}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}''}^+, \{n_{\mathbf{q}}\}, t \right) - F_G''^* e^{-iq''_z z} \sqrt{n_{\mathbf{q}''}} f_w \left(z, p_z \mp \frac{\hbar(q'_z \mp q''_z)}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}''}^-, \{n_{\mathbf{q}}\}, t \right) \right. \\
& \quad \left. - F_G'' e^{iq''_z z} \sqrt{n_{\mathbf{q}''}} f_w \left(z, p_z \mp \frac{\hbar(q'_z \mp q''_z)}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}''}^-, \{n_{\mathbf{q}}\}, t \right) + F_G''^* e^{-iq''_z z} \sqrt{n_{\mathbf{q}''}} + 1 f_w \left(z, p_z \mp \frac{\hbar(q'_z \pm q''_z)}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}''}^+, \{n_{\mathbf{q}}\}, t \right) \right\}. \quad (5)
\end{aligned}$$

Accordingly we refer to the separate equations as Eqs. (5[±]). On this stage we approximate the equations by neglecting all SOD elements on the right. The only elements in Eq. (5[±]) which are not SOD are obtained from the second and fourth terms on the right in the case $\mathbf{q}'' = \mathbf{q}'$. In particular the factor $\sqrt{n_{\mathbf{q}''}}$ becomes $\sqrt{n_{\mathbf{q}'} + 1}$ as by default the number of phonons in \mathbf{q}' mode is raised by unity. Similarly, in Eq. (5⁻) the first and third terms on the right recover diagonal elements if $\mathbf{q}'' = \mathbf{q}'$. The factor $\sqrt{n_{\mathbf{q}''} + 1}$ becomes $\sqrt{n_{\mathbf{q}'}}$ since the number of phonons in \mathbf{q}' mode is lowered by unity.

We will make use of the integral forms of the approximated equations. According to Appendix A the integral formulation is obtained with the help of the characteristics of

the Liouville operators in Eq. (5). These are Newton's trajectories, Eq. (A1), initialized by the time and phase space variables which identify the left-hand sides of Eqs. (5[±]). Thus the particular trajectories are initialized by $(z, p_z \mp \hbar q'_z / 2, t)$

$$z^{\mp}(t') = z - \frac{1}{m} \int_{t'}^t p_z^{\mp}(\tau) d\tau,$$

$$p_z^{\mp}(t') = p_z \mp \frac{\hbar q'_z}{2} - eE(t - t') = p_z(t') \mp \frac{\hbar q'_z}{2}. \quad (6)$$

As the electron-phonon system is initially decoupled, the initial conditions for f_{FOD}^{\pm} are zero:

$$\begin{aligned}
f_w \left(z, p_z \mp \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}'}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t \right) & = F_G^{\mp}(\mathbf{q}') \sqrt{n_{\mathbf{q}'} + \frac{1}{2} \pm \frac{1}{2}} \int_0^t dt' e^{\mp i\omega_{\mathbf{q}'}(t-t')} e^{\mp iq'_z z^{\mp}(t')} \{ \mp f_w(z^{\mp}(t'), p_z(t'), \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t') \\
& \quad \pm f_w(z^{\mp}(t'), p_z(t') \mp \hbar q'_z, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^{\pm}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^{\pm}, t') \}. \quad (7)
\end{aligned}$$

Here $F_G^+ = F_G$, $F_G^- = F_G^*$ and, consistently with Eq. (6), $p_z(t') = p_z - eE(t - t')$.

B. Inhomogeneous Levinson equation

A substitution of Eq. (7) into Eq. (4) yields an equation which contains only diagonal elements of the GWF:

$$\begin{aligned}
& \left(\frac{\partial}{\partial t} + \frac{p_z}{m} \nabla_z + eE \nabla_{p_z} \right) f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t) \\
& = 2 \operatorname{Re} \left(\sum_{\mathbf{q}'} |F_G(\mathbf{q}')|^2 \int_0^t dt' \{ (n_{\mathbf{q}'}) \right. \\
& \quad + 1 \} e^{iq'_z z} e^{-i\omega_{\mathbf{q}'}(t-t')} e^{-iq'_z z^-(t')} [f_w(z^-(t'), (p_z - \hbar q'_z)(t'), \\
& \quad \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, t') - f_w(z^-(t'), p_z(t'), \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t')] \\
& \quad - n_{\mathbf{q}'} e^{-iq'_z z} e^{i\omega_{\mathbf{q}'}(t-t')} e^{iq'_z z^+(t')} [f_w(z^+(t'), p_z(t'), \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t') \\
& \quad \left. - f_w(z^+(t'), p_z(t') + \hbar q'_z, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^-, t')] \right\}. \quad (8)
\end{aligned}$$

The arguments of the exponent are evaluated with the help of Eq. (6):

$$\begin{aligned}
& \pm q'_z z^{\mp} \mp \omega_{\mathbf{q}'}(t - t') \mp q'_z z^{\mp}(t') \\
& = - \int_{t'}^t \left[\frac{q'_z}{m} \left(p_z - eE(t - \tau) \mp \frac{\hbar q'_z}{2} \right) \mp \omega_{\mathbf{q}'} \right] d\tau \\
& = \mp \int_{t'}^t \frac{1}{\hbar} [\epsilon(p_z(\tau)) - \epsilon(p_z(\tau) \mp \hbar q'_z) \mp \hbar \omega_{\mathbf{q}'}] d\tau.
\end{aligned}$$

Furthermore, we modify Eq. (8) by switching the sign of \mathbf{q}' in the last row (for this we rely on the symmetry of $\omega_{\mathbf{q}'}$ and F_G) and by introducing the variable $p'_z = p_z - \hbar q'_z$.

The electron Wigner function (3) is obtained with the help of the assumption that the phonon system remains in equilibrium during the evolution. Formally this means that the variables in the diagonal elements can be separated as follows:

$$f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}'}\}, t') = f_w(z, p_z, t') \prod_{\mathbf{q}} P_{eq}(n_{\mathbf{q}}). \quad (9)$$

Here $P_{eq}(n_{\mathbf{q}})$ is the equilibrium probability for finding $n_{\mathbf{q}}$ phonons in mode \mathbf{q} . The mean equilibrium phonon number $n(\mathbf{q})$ is given by the Bose-Einstein distribution:

$$n(\mathbf{q}) = \sum_{n_{\mathbf{q}}=0}^{\infty} n_{\mathbf{q}} P_{eq}(n_{\mathbf{q}}), \quad \sum_{n_{\mathbf{q}}=0}^{\infty} P_{eq}(n_{\mathbf{q}}) = 1. \quad (10)$$

We replace Eq. (9) into the modified equation (8) and perform the trace operation. The phonon coordinates are encountered with the help of the equalities

$$n(\mathbf{q}) + \frac{1}{2} \mp \frac{1}{2} = \sum_{n_{\mathbf{q}}} \left(n_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2} \right) P_{eq}(n_{\mathbf{q}} \pm 1). \quad (11)$$

An equation of Levinson type is obtained:

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \frac{p_z}{m} \nabla_z + eE \nabla_{p_z} \right) f_w(z, p_z, t) \\ &= \sum_{\mathbf{q}'_{\perp}, p'_z} \int_0^t dt' \{ S(p_z, p'_z, \mathbf{q}'_{\perp}, t, t') f_w(z^-(t'), p_z^-(t'), t') \\ & \quad - S(p'_z, p_z, \mathbf{q}'_{\perp}, t, t') f_w(z^-(t'), p_z^-(t'), t') \}, \end{aligned} \quad (12)$$

$$\begin{aligned} S(p_z, p'_z, \mathbf{q}'_{\perp}, t, t') &= 2 |F_G(\mathbf{q}')|^2 \\ & \times \left[n(\mathbf{q}) \cos \left(\int_{t'}^t \frac{[\epsilon(p_z(\tau)) - \epsilon(p'_z(\tau)) - \hbar \omega_{\mathbf{q}'}] d\tau}{\hbar} \right) \right. \\ & \left. + [n(\mathbf{q}) + 1] \cos \left(\int_{t'}^t \frac{[\epsilon(p_z(\tau)) - \epsilon(p'_z(\tau)) + \hbar \omega_{\mathbf{q}'}] d\tau}{\hbar} \right) \right], \end{aligned} \quad (13)$$

which describes the inhomogeneous evolution of carriers excited in a quantum wire. The discussion of its properties is postponed to Sec. V.

The physically transparent manner of the derivation of Eq. (12) encourages us to make a further step and to take into account the next level in the hierarchy of linked GWF elements.

IV. TRUNCATION AT THE SOD LEVEL

A. Closure of the equation for f_{FOD}^+

We first consider Eq. (5⁺) and look for a criteria by which to retain also certain SOD elements on the right-hand side of the equation. Four types of such elements, shortly denoted by f_{SOD}^{++} , f_{SOD}^{+-} , f_{SOD}^{-+} , and f_{SOD}^{--} , appear consecutively in the terms on the right. In this notation the comma separates the left from the right basis so that ++ means two extra phonons in states \mathbf{q}' and \mathbf{q}'' in the left basis, etc. f_{SOD}^{+-} and f_{SOD}^{-+} , which give rise to the only diagonal elements, have already been used above. We then analyze the SOD elements of the first and third terms: f_{SOD}^{++} and f_{SOD}^{--} . They contain two extra phonons in the left basis. The corresponding equations of motion involve a frequency of $i2\omega$ added to the Liouville operator on the left-hand side. As compared to the diagonal elements, these SOD elements oscillate rapidly in time. A straightforward application of the RPA requires them to be neglected. Then the second and fourth terms remain to be combined to give additional corrections to the diagonal terms. However, a careful analysis shows that also f_{SOD}^{+-} and f_{SOD}^{-+} give contributions: it is correct to compare elements linked within an equation. Jumps in the hierarchy such as, e.g., a comparison between SOD and diagonal elements can lead to erroneous conclusions.

We evaluate consecutively the contributions from the SOD elements to the right-hand side of Eq. (5⁺). The corresponding equations of motion in general introduce third off-diagonal elements. We follow the same strategy for approximation of the right-hand sides of these equations. Namely, we consider only special cases where third off-diagonal elements reduce to FOD elements. Then the SOD equations are solved and replaced in Eq. (5⁺). An equation is obtained which contains FOD elements only. This equation along with the counterpart obtained from Eq. (5⁻) is used to close Eq. (4). In what follows we need to assume a constant phonon frequency $\omega_{\mathbf{q}} = \omega$.

1. Contribution from f_{SOD}^{++}

We begin with the equation of motion of f_{SOD}^{++} :

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \frac{p_z - \hbar(q'_z + q''_z)/2}{m} \nabla_z + eE \nabla_{p_z} + i2\omega \right) f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+ \}_{\mathbf{q}''}^+, \{ n_{\mathbf{q}} \}, t \right) \\ &= + \sum_{\mathbf{q}'''} \left\{ F_G(\mathbf{q}''') e^{iq''_z z} \sqrt{n_{\mathbf{q}'''}} + 1 f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z + q'''_z)}{2}, \{ \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+ \}_{\mathbf{q}''}^+ \}_{\mathbf{q}'''}^+, \{ n_{\mathbf{q}} \}, t \right) \right. \\ & \quad - F_G^*(\mathbf{q}''') e^{-iq''_z z} \sqrt{n_{\mathbf{q}'''}} f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z - q'''_z)}{2}, \{ \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+ \}_{\mathbf{q}''}^+ \}_{\mathbf{q}'''}^-, \{ n_{\mathbf{q}} \}, t \right) \\ & \quad - F_G(\mathbf{q}''') e^{iq''_z z} \sqrt{n_{\mathbf{q}'''}} f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z - q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+ \}_{\mathbf{q}''}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^-, t \right) \\ & \quad \left. + F_G^*(\mathbf{q}''') e^{-iq''_z z} \sqrt{n_{\mathbf{q}'''}} + 1 f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z + q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+ \}_{\mathbf{q}''}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^+, t \right) \right\}. \end{aligned} \quad (14)$$

We approximate this equation by neglecting all terms but those containing FOD elements. Only two terms on the right can give rise to FOD elements. These are the second and fourth terms, provided that $\mathbf{q}''' = \mathbf{q}''$ or $\mathbf{q}''' = \mathbf{q}'$. The equation is integrated with the help of a trajectory obtained from Eq.

(6) for the initialization point $(z, p_z - \frac{\hbar(q'_z + q''_z)}{2}, t)$ identifying the Liouville operator in Eq. (14). The free term is zero, as the electron-phonon system is initially decoupled:

$$\begin{aligned}
& F_G(\mathbf{q}'') e^{iq''_z z} f_w \left(z, p_z - \frac{\hbar(q'_z + q''_z)}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}^+\}_{\mathbf{q}''}, \{n_{\mathbf{q}}\}, t \right) \\
&= - \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{iq''_z z} e^{-iq''_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''} + 1} f_w \left(z(t'), p_z(t') - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t' \right) \\
&\quad - \int_0^t dt' F_G^*(\mathbf{q}') F_G(\mathbf{q}'') e^{iq''_z z} e^{-iq'_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}'} + 1} f_w \left(z(t'), p_z(t') - \frac{\hbar q''_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^+, \{n_{\mathbf{q}}\}, t' \right) \\
&\quad + \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{iq''_z z} e^{-iq''_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''}} f_w \left(z(t'), p_z(t') - \frac{\hbar(q'_z + 2q''_z)}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}^+\}_{\mathbf{q}''}, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^+, t' \right) \\
&\quad + \int_0^t dt' F_G^*(\mathbf{q}') F_G(\mathbf{q}'') e^{iq''_z z} e^{-iq'_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}'}} f_w \left(z(t'), p_z(t') - \frac{\hbar(2q'_z + q''_z)}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}^+\}_{\mathbf{q}''}, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^+, t' \right). \quad (15)
\end{aligned}$$

Equation (15) can be replaced in Eq. (5⁺), so that its right-hand side appears as a correction attached to the right-hand side of Eq. (5⁺). We evaluate the oscillations in time of the correction terms. However, the integro-differential form is not convenient for an analysis in the time domain. In particular the left-hand side of Eq. (5⁺) depends on $i\omega$ while the correction terms depend on $e^{-i2\omega(t-t')}$. Convenient for this purpose is the integral form of the equation, which appears to be Eq. (7⁺) with additional terms on the right-hand side arising from Eq. (15). The corrections due to these terms are additive, so that their contributions can be evaluated separately. We begin with the first term in Eq. (15) rewritten so

that the q''_z dependent arguments of the exponents are expressed in terms of electron energies:

$$\begin{aligned}
& q''_z z - q''_z z(t') \\
&= \int_{t'}^t \frac{\epsilon(p_z(\tau) - \hbar q'_z/2) - \epsilon(p_z(\tau) - \hbar q'_z/2 - \hbar q''_z)}{\hbar} d\tau. \quad (16)
\end{aligned}$$

For notational convenience we denote the energy difference in the numerator by $\Delta\epsilon(\tau)$. The term under consideration gives rise to the following contribution to the right-hand side of Eq. (7⁺):

$$\begin{aligned}
& f_w \left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t \right) = \dots - \sum_{\mathbf{q}''} (n_{\mathbf{q}''} + 1) |F_G(\mathbf{q}'')|^2 \int_0^t dt' \int_0^{t'} dt'' e^{-i\omega(t-t')} e^{-i2\omega(t'-t'')} e^{i \int_{t''}^{t'} \Delta\epsilon(\tau) d\tau} f_w \left(z(t'), t'', p_z(t'') \right. \\
&\quad \left. - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t'' \right), \quad (17)
\end{aligned}$$

where $z(t', t'')$ is expressed with the help of Eq. (6),

$$z(t', t'') = z^-(t') - \frac{1}{m} \int_{t''}^{t'} \left(p_z(\tau) - \frac{\hbar(q'_z + q''_z)}{2} \right) d\tau. \quad (18)$$

Equation (17) has a convenient form for analysis of the time dependence. The time integrals can be transformed with the help of the equality $\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$:

$$\begin{aligned}
& \int_0^t dt' \int_0^{t'} dt'' e^{-i\omega(t-t')} e^{-i2\omega(t'-t'')} e^{i \int_{t''}^{t'} \Delta\epsilon(\tau) d\tau} f_w \\
&= \int_0^t dt'' e^{-i\omega(t-t'')} \int_{t''}^t dt' e^{i \int_{t''}^{t'} [\Delta\epsilon(\tau) - \hbar\omega] d\tau} f_w. \quad (19)
\end{aligned}$$

Next the inner integral is approximated by taking the classical limit $\hbar \rightarrow 0$. The limit is discussed in detail in Appendix

B. It gives rise to a δ function and a principle value according to the formal relation

$$\lim_{\hbar \rightarrow 0} \frac{1}{\hbar} \int_0^t d\tau e^{i\epsilon\tau/\hbar} = \pi\delta(\epsilon) + \text{VP} \frac{i}{\epsilon}.$$

We note that this limit conveniently sets t' to t'' so that $z(t', t'')$ in f_w , Eq. (17), becomes $z^-(t'')$. If only the δ function is accounted for, Eq. (17) takes the form

$$\begin{aligned} f_w\left(z, p_z - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t\right) \\ = \dots - \int_0^t dt'' e^{-i\omega(t-t'')} \sum_{\mathbf{q}''} (n_{\mathbf{q}''} + 1) |F_G(\mathbf{q}'')|^2 \pi \hbar \delta\left(\epsilon\left(p_z(t'') - \frac{\hbar q'_z}{2}\right) - \epsilon\left(p_z(t'') - \frac{\hbar q'_z}{2} - \hbar q''_z\right) - \hbar\omega\right) f_w\left(z(t''), p_z(t'') - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t''\right). \end{aligned} \quad (20)$$

This equation is of the type (A3), which along with Eq. (A5) have a common differential counterpart given by Eq. (A4), Appendix A. In other words, if we take the time derivative of Eq. (20), we obtain Eq. (5⁺) with an additional term $\gamma_e^{f_{\text{FOD}}}$ appearing on the right-hand side of the equation. If transferred to the left this term gives rise to the correction

$$\begin{aligned} F_G(\mathbf{q}'') e^{iq''_z z} f_w\left(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^-, t\right) \\ = - \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{iq''_z z} e^{-iq''_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''}} f_w\left(z(t'), p_z(t') - \frac{\hbar(q'_z - 2q''_z)}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}^+\}_{\mathbf{q}''}^-, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^-, t'\right) \\ - \int_0^t dt' F_G^*(\mathbf{q}') F_G(\mathbf{q}'') e^{iq''_z z} e^{-iq'_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''} + 1} f_w\left(z(t'), p_z(t') + \frac{\hbar q''_z}{2}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^-, t'\right) \\ + \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{iq''_z z} e^{-iq''_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''}} f_w\left(z(t'), p_z(t') - \frac{\hbar q'_z}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}, t'\right) \\ + \int_0^t dt' F_G^*(\mathbf{q}') F_G(\mathbf{q}'') e^{iq''_z z} e^{-iq'_z z(t')} e^{-i2\omega(t-t')} \sqrt{n_{\mathbf{q}''} + 1} f_w\left(z(t'), p_z(t') - \frac{\hbar(2q'_z - q''_z)}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{\{n_{\mathbf{q}}\}_{\mathbf{q}''}^-\}_{\mathbf{q}'}^+, t'\right). \end{aligned}$$

Only the third term on the right survives after the RPA. Taking into account the particular trajectory $z(t')$ we can express $q''_z z - q'_z z(t')$ in the exponent as

$$- \int_{t'}^t \frac{\epsilon(p_z(\tau) - \hbar q'_z/2) - \epsilon(p_z(\tau) - \hbar q'_z/2 + \hbar q''_z)}{\hbar} d\tau. \quad (22)$$

$$\begin{aligned} \gamma_e\left(p_z - \frac{\hbar q'_z}{2}\right) = \sum_{\mathbf{q}''} (n_{\mathbf{q}''} + 1) |F_G(\mathbf{q}'')|^2 \pi \hbar \delta\left(\epsilon\left(p_z - \frac{\hbar q'_z}{2}\right) - \epsilon\left(p_z - \frac{\hbar q'_z}{2} - \hbar q''_z\right) - \hbar\omega\right) \end{aligned} \quad (21)$$

added to the Liouville operator in the brackets of Eq. (5⁺). We note that the summation over \mathbf{q}'' involves only positive contributions to γ_e . The imaginary term with the principal value affects the phonon frequency—an effect known as a polaron shift in the energies. Here this effect is neglected.

Consider the rest of the terms in Eq. (15). The prefactor of the third term in Eq. (15) can be evaluated in the same way leading to Eq. (20). However, now the corresponding GWF element depends on \mathbf{q}'_z and thus would contribute as a complex quantity to the sum in Eq. (5⁺). The same holds for the GWF elements in the second and fourth terms, which, moreover, depend on the oscillatory prefactor $e^{i(q''_z - q'_z)z}$. By referring to the RPA we can neglect these three terms.

Essentially the same steps will be applied for the rest of the terms. Next we evaluate the contribution from the third term since the derivations closely follow the steps already considered.

2. Contribution from $f_{\text{SOD}}^{+\bar{-}}$

We write down the equation for $f_w(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}^+, \{n_{\mathbf{q}}\}_{\mathbf{q}''}^-, t)$ and consider only the FOD elements which appear on the right. The equation is integrated with the help of a trajectory initialized by the phase space variables $(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, t)$. The solution is obtained explicitly in terms of FOD elements:

This differs from Eq. (16) by the leading sign and the sign of q''_z . As before we denote the energy difference by $\Delta\epsilon(\tau)$ and evaluate the contribution of the term to the integral form of Eq. (5⁺). An expression is obtained, which differs from Eq. (17) in the following: (i) the factor $(n_{\mathbf{q}''} + 1)$ is replaced by $n_{\mathbf{q}''}$; (ii) $\Delta\epsilon(\tau)$ is updated according to Eq. (22); (iii) $z(t', t'')$ is updated from Eq. (18) by changing the sign of q''_z from

plus to minus. The evaluation of the time integrals follows exactly Eq. (19). By taking the classical limit and following the arguments leading to Eq. (21), we obtain the term

$$\gamma_a \left(p_z - \frac{\hbar q'_z}{2} \right) = \sum_{\mathbf{q}''} n_{\mathbf{q}''} |F_G(\mathbf{q}'')|^2 \pi \hbar \delta \left(\epsilon \left(p_z - \frac{\hbar q'_z}{2} \right) - \epsilon \left(p_z - \frac{\hbar q''_z}{2} + \hbar q''_z \right) + \hbar \omega \right), \quad (23)$$

which must be added to the Liouville operator in Eq. (5⁺).

The phonon energy is now added to $\Delta\epsilon$ due to the minus sign in front of Eq. (22).

3. Correction from f_{SOD}^{+-}

The second term in Eq. (5⁺) already provided a diagonal element. We pursue what additional contribution δf_{SOD}^{+-} can be obtained from the corresponding equation of motion. Apparently δf_{SOD}^{+-} is

$$(1 - \delta_{\mathbf{q}', \mathbf{q}''}) f_w \left(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^- \}, \{ n_{\mathbf{q}} \}, t \right),$$

so that the equation of motion assumes that $\mathbf{q}' \neq \mathbf{q}''$:

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \frac{p_z - \hbar(q'_z - q''_z)/2}{m} \nabla_z + eE \nabla_{p_z} \right) \delta f_{SOD}^{+-} \left(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^- \}, \{ n_{\mathbf{q}} \}, t \right) \\ &= + \sum_{\mathbf{q}'''} \left\{ F_G(\mathbf{q}''') e^{iq''_z z} \sqrt{n_{\mathbf{q}'''} + 1} f_w \left(z, p_z - \frac{\hbar(q'_z - q''_z + q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^- \}, \{ n_{\mathbf{q}} \}, t \right) - F_G^*(\mathbf{q}''') e^{-iq''_z z} \sqrt{n_{\mathbf{q}'''} f_w} \left(z, p_z \right. \right. \\ & \quad \left. \left. - \frac{\hbar(q'_z - q''_z - q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^- \}, \{ n_{\mathbf{q}} \}, t \right) - F_G(\mathbf{q}''') e^{iq''_z z} \sqrt{n_{\mathbf{q}'''} f_w} \left(z, p_z - \frac{\hbar(q'_z - q''_z - q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^- \}, t \right) \right. \\ & \quad \left. + F_G^*(\mathbf{q}''') e^{-iq''_z z} \sqrt{n_{\mathbf{q}'''} + 1} f_w \left(z, p_z - \frac{\hbar(q'_z - q''_z + q'''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}_{\mathbf{q}'''}^+ \}, t \right) \right\}. \quad (24) \end{aligned}$$

The four terms on the right-hand side contain FOD elements obtained, respectively, by the combinations $\mathbf{q}''' = \mathbf{q}''$, $\mathbf{q}''' = \mathbf{q}'$, $\mathbf{q}''' = \mathbf{q}''$, and $\mathbf{q}''' = \mathbf{q}'$. We recall that in this case $n_{\mathbf{q}'''}$ must be updated according to the actual number of phonons in modes

\mathbf{q}' or \mathbf{q}'' , respectively. The reduced equation is integrated with the help of the trajectory $(z(t'), p_z(t'))$ initialized by the phase space variables $(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, t)$. The correction δf_{SOD}^{+-} is expressed in terms of FOD elements:

$$\begin{aligned} & F_G^*(\mathbf{q}'') e^{-iq''_z z} \delta f_{SOD}^{+-} \left(z, p_z - \frac{\hbar(q'_z - q''_z)}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^- \}, \{ n_{\mathbf{q}} \}, t \right) \\ &= + \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{-iq''_z z} e^{iq''_z z(t')} \sqrt{n_{\mathbf{q}''} f_w} \left(z(t'), p_z(t') - \frac{\hbar q'_z}{2}, \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}, t' \right) \\ & \quad - \int_0^t dt' F_G^*(\mathbf{q}') F_G^*(\mathbf{q}'') e^{-iq''_z z} e^{-iq'_z z(t')} \sqrt{n_{\mathbf{q}'} + 1} f_w \left(z(t'), p_z(t') + \frac{\hbar q''_z}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}, t' \right) \\ & \quad - \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{-iq''_z z} e^{iq''_z z(t')} \sqrt{n_{\mathbf{q}''} f_w} \left(z(t'), p_z(t') + \hbar q''_z - \frac{\hbar q'_z}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, t' \right) \\ & \quad + \int_0^t dt' F_G^*(\mathbf{q}'') F_G^*(\mathbf{q}') e^{-iq''_z z} e^{-iq'_z z(t')} \sqrt{n_{\mathbf{q}'} + 1} f_w \left(z(t'), p_z(t') - \hbar q'_z + \frac{\hbar q''_z}{2}, \{ \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, \{ n_{\mathbf{q}} \}_{\mathbf{q}''}^-, \{ n_{\mathbf{q}} \}_{\mathbf{q}'}^+, t' \right). \quad (25) \end{aligned}$$

We evaluate the contribution of the first term to Eq. (7). As before the arguments of the exponents introduce the energy difference $\Delta\epsilon(\tau)$,

$$\begin{aligned} q_z'' z(t') - q_z' z \\ = \int_{t'}^t \frac{\epsilon(p_z(\tau) - \hbar q_z'/2) - \epsilon(p_z(\tau) - \hbar q_z'/2 + \hbar q_z'')}{\hbar} d\tau, \end{aligned} \quad (26)$$

under the time integral. This contribution is obtained as follows:

$$\begin{aligned} f_w\left(z, p_z - \frac{\hbar q_z'}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t\right) = \dots \\ - \sum_{\mathbf{q}''} n_{\mathbf{q}''} |F_G'|^2 \int_0^t dt' \int_0^{t'} dt'' e^{-i\omega(t-t')} e^{i\int_{t''}^{t'} \Delta\epsilon(\tau) d\tau} \\ \times f_w\left(z(t', t''), p_z(t'') - \frac{\hbar q_z'}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t''\right), \end{aligned} \quad (27)$$

where

$$z(t', t'') = z^-(t') - \frac{1}{m} \int_{t''}^{t'} \left(p_z(\tau) - \frac{\hbar(q_z' - q_z'')}{2} \right) d\tau. \quad (28)$$

The time integrals are processed accordingly:

$$\begin{aligned} \int_0^t dt' \int_0^{t'} dt'' e^{-i\omega(t-t')} e^{i\int_{t''}^{t'} \Delta\epsilon(\tau) d\tau} f_w \\ = \int_0^t dt'' e^{-i\omega(t-t'')} \int_{t''}^t dt' e^{i\int_{t''}^{t'} [\Delta\epsilon(\tau) + \hbar\omega] d\tau} f_w. \end{aligned} \quad (29)$$

After taking the classical limit in the inner integral and neglecting the principal value we obtain the contribution to the Liouville operator in Eq. (5⁺):

$$\begin{aligned} \gamma_a\left(p_z - \frac{\hbar q_z'}{2}\right) = \sum_{\mathbf{q}''} n_{\mathbf{q}''} |F_G(\mathbf{q}'')|^2 \pi \hbar \delta\left(\epsilon\left(p_z - \frac{\hbar q_z'}{2}\right) \right. \\ \left. - \epsilon\left(p_z - \frac{\hbar q_z'}{2} + \hbar q_z''\right) + \hbar\omega\right). \end{aligned}$$

The rest of the terms in Eq. (25) are neglected with the help of the RPA.

4. Correction from δf_{SOD}^{*+}

The correction δf_{SOD}^{*+} originating with the fourth term in Eq. (7) satisfies the equation

$$\begin{aligned} \left(\frac{\partial}{\partial t} + \frac{p_z - \hbar(q_z' + q_z'')/2}{m} \nabla_z + eE \nabla_{p_z} \right) \delta f_{SOD}^{*+}\left(z, p_z - \frac{\hbar(q_z' + q_z'')}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, t\right) \\ = + \sum_{\mathbf{q}'''} \left\{ F_G(\mathbf{q}''') e^{iq_z'' z} \sqrt{n_{\mathbf{q}''}} + 1 f_w\left(z, p_z - \frac{\hbar(q_z' + q_z'' + q_z''')}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}\}^+, \{n_{\mathbf{q}}\}_{\mathbf{q}''}, t\right) - F_G^*(\mathbf{q}''') e^{-iq_z'' z} \sqrt{n_{\mathbf{q}''}} f_w\left(z, p_z \right. \right. \\ \left. \left. - \frac{\hbar(q_z' + q_z'' - q_z''')}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}\}^+, \{n_{\mathbf{q}}\}_{\mathbf{q}''}, t\right) - F_G(\mathbf{q}''') e^{iq_z'' z} \sqrt{n_{\mathbf{q}''}} f_w\left(z, p_z - \frac{\hbar(q_z' + q_z'' - q_z''')}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}\}^+, \{\{n_{\mathbf{q}}\}_{\mathbf{q}''}\}^-, t\right) \right. \\ \left. + F_G^*(\mathbf{q}''') e^{-iq_z'' z} \sqrt{n_{\mathbf{q}''}} + 1 f_w\left(z, p_z - \frac{\hbar(q_z' + q_z'' + q_z''')}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}''}\}^+, t\right) \right\} \end{aligned} \quad (30)$$

under the condition $\mathbf{q}' \neq \mathbf{q}''$. The four terms on the right-hand side contain FOD elements obtained, respectively, by the combinations $\mathbf{q}''' = \mathbf{q}''$, $\mathbf{q}''' = \mathbf{q}'$, $\mathbf{q}''' = \mathbf{q}''$, and $\mathbf{q}''' = \mathbf{q}'$. The equation is integrated with the help of a trajectory initialized by $(z, p_z - \frac{\hbar(q_z' + q_z'')}{2}, t)$:

$$\begin{aligned} F_G^*(\mathbf{q}'') e^{-iq_z'' z} \delta f_{SOD}^{*+}\left(z, p_z - \frac{\hbar(q_z' + q_z'')}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, t\right) \\ = + \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{-iq_z'' z} e^{iq_z'' z(t')} \sqrt{n_{\mathbf{q}''}} + 1 f_w\left(z(t'), p_z(t') - \hbar q_z'' - \frac{\hbar q_z'}{2}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}\}^+, \{\{n_{\mathbf{q}}\}_{\mathbf{q}''}\}^+, t'\right) \\ - \int_0^t dt' F_G^*(\mathbf{q}') F_G^*(\mathbf{q}'') e^{-iq_z'' z} e^{-iq_z'' z(t')} \sqrt{n_{\mathbf{q}'}} + 1 f_w\left(z(t'), p_z(t') - \frac{\hbar q_z''}{2}, \{n_{\mathbf{q}}\}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}''}\}^+, t'\right) \\ - \int_0^t dt' |F_G(\mathbf{q}'')|^2 e^{-iq_z'' z} e^{iq_z'' z(t')} \sqrt{n_{\mathbf{q}''}} + 1 f_w\left(z(t'), p_z(t') - \frac{\hbar q_z'}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t'\right) \\ + \int_0^t dt' F_G^*(\mathbf{q}'') F_G^*(\mathbf{q}') e^{-iq_z'' z(t')} e^{-iq_z'' z} \sqrt{n_{\mathbf{q}'}} + 1 f_w\left(z(t'), p_z(t') - \hbar q_z' - \frac{\hbar q_z''}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{\{n_{\mathbf{q}}\}_{\mathbf{q}'}\}^+, t'\right). \end{aligned} \quad (31)$$

An application of the RPA filters all terms but the third. Taking into account the particular form of the trajectory $z(t')$ we obtain the exponential factor $-q_z''z + q_z''z(t')$ expressed in terms of electron energies:

$$-\int_{t'}^t \frac{[\epsilon(p_z(\tau) - \hbar q_z'/2) - \epsilon(p_z(\tau) - \hbar q_z'/2 - \hbar q_z'')]d\tau}{\hbar}. \quad (32)$$

This expression differs from Eq. (26) by the leading sign and the sign of q_z'' . The contribution of $\delta f_{SOD}^{+,+}$ to the FOD element accounted in the integral form of Eq. (5⁺) gives rise to an expression which differs from Eq. (27) in the following: (i) the factor $n_{\mathbf{q}''}$ in front of $|F_G|^2$ becomes $(n_{\mathbf{q}''}+1)$; (ii) the

energy difference in the exponent is updated according to Eq. (32); (iii) $z(t', t'')$ is updated according to Eq. (28) by changing the sign of q_z'' from plus to minus. Processing the time integrals as in Eq. (29) and repeating the same steps we obtain the additive term

$$\gamma_e \left(p_z - \frac{\hbar q_z'}{2} \right) = \sum_{\mathbf{q}''} (n_{\mathbf{q}''} + 1) |F_G(\mathbf{q}'')|^2 \pi \hbar \delta \left(\epsilon \left(p_z - \frac{\hbar q_z'}{2} \right) - \epsilon \left(p_z - \frac{\hbar q_z'}{2} - \hbar q_z'' \right) - \hbar \omega \right),$$

which appears in the bracket on the left-hand side of Eq. (5⁺). By denoting $\gamma = 2(\gamma_a + \gamma_e)$ we are ready to formulate the truncated equation for the first FOD element:

$$\left[\frac{\partial}{\partial t} + \frac{p_z - \hbar q_z'/2}{m} \nabla_z + eE \nabla_{p_z} + \gamma \left(p_z - \frac{\hbar q_z'}{2} \right) + i\omega \right] f_w \left(z, p_z - \frac{\hbar q_z'}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t \right) = F_G^*(\mathbf{q}') e^{-iq_z'z} \sqrt{n_{\mathbf{q}'}} + 1 [f_w(z, p_z - \hbar q_z', \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, t) - f_w(z, p_z, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}, t)]. \quad (33)$$

B. Closure of the equation for f_{FOD}^-

The right-hand side of Eq. (5⁻) refers to SOD elements, whose number of phonons in mode \mathbf{q}' of the left basis is reduced by 1. These elements are denoted by $f_{SOD}^{+,+}$, $f_{SOD}^{+,+}$, $f_{SOD}^{+,+}$, and $f_{SOD}^{+,+}$ according to the order of their appearance the right. Diagonal elements are provided by the first and the third terms $f_{SOD}^{+,+}$ and $f_{SOD}^{+,+}$. Accordingly, we pursue the equations of motion of the corrections $\delta f_{SOD}^{+,+}$ and $\delta f_{SOD}^{+,+}$ for appropriate contributions to Eq. (5⁻). The equations for the remaining two terms—namely, $f_{SOD}^{+,+}$ and $f_{SOD}^{+,+}$ —are also explored for such contributions. The analysis follows the same steps of retaining the FOD elements on the right-hand side of the corresponding equations and applying the RPA.

Next the contributions obtained are approximated by taking the classical limit. We skip the long but straightforward algebraic steps and summarize the terms added to the Liouville operator in Eq. (5⁻) by the following scheme:

$$f_{SOD}^{+,+} \rightarrow \gamma_e \left(p_z + \frac{\hbar q_z'}{2} \right), f_{SOD}^{+,+} \rightarrow \gamma_a \left(p_z + \frac{\hbar q_z'}{2} \right),$$

$$f_{SOD}^{+,+} \rightarrow \gamma_e \left(p_z + \frac{\hbar q_z'}{2} \right), f_{SOD}^{+,+} \rightarrow \gamma_a \left(p_z + \frac{\hbar q_z'}{2} \right).$$

Collecting all terms into $\gamma = 2(\gamma_a + \gamma_e)$, we formulate the truncated equation for the second FOD element:

$$\left[\frac{\partial}{\partial t} + \frac{p_z + \hbar q_z'/2}{m} \nabla_z + eE \nabla_{p_z} + \gamma \left(p_z + \frac{\hbar q_z'}{2} \right) - i\omega \right] f_w \left(z, p_z + \frac{\hbar q_z'}{2}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t \right) = F_G(\mathbf{q}') e^{iq_z'z} \sqrt{n_{\mathbf{q}'}} [f_w(z, p_z, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}, t) - f_w(z, p_z + \hbar q_z', \{n_{\mathbf{q}}\}_{\mathbf{q}'}, \{n_{\mathbf{q}}\}_{\mathbf{q}'}, t)]. \quad (34)$$

C. Inhomogeneous Barker-Ferry equation

Equations (33) and (34) generalize Eq. (5). Aiming at a closed equation for the electron Wigner function we follow essentially the same steps used to obtain the Levinson equation. The corresponding integral equations resemble Eq. (7) corrected by the exponents $e^{-\int_{t'}^t \gamma(p_z(\tau) - \hbar q_z'/2) d\tau}$, which appear

on the right-hand sides. A replacement into Eq. (4) gives rise to a generalization of Eq. (8), where $e^{-\int_{t'}^t \gamma(p_z(\tau) - \hbar q_z'/2) d\tau}$ is attached to the exponents of the second row and $e^{-\int_{t'}^t \gamma(p_z(\tau) + \hbar q_z'/2) d\tau}$ is attached to the exponents of the last row. In the latter we switch the sign of \mathbf{q}' , introduce the variable p_z' , and perform the trace operation. However, now, the

evaluation of the trace is not as straightforward as in the Levinson case. The reason is that γ brings a nonlinear dependence from the phonon degrees of freedom so that Eq. (11) can be applied after additional considerations of the phonon system. We postpone the discussion of this for the next section and formulate the inhomogeneous Barker-Ferry model obtained:

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \frac{p_z}{m} \nabla_z + eE \nabla_{p_z} \right) f_w(z, p_z, t) \\ &= \sum_{\mathbf{q}'_{\perp}, p'_z} \int_0^t dt' \{ S(p_z, p'_z, \mathbf{q}'_{\perp}, t, t') f_w(z^-(t'), p_z^-(t'), t') \\ & \quad - S(p'_z, p_z, \mathbf{q}'_{\perp}, t, t') f_w(z^-(t'), p_z^-(t'), t') \}, \end{aligned} \quad (35)$$

where

$$\begin{aligned} S(p_z, p'_z, \mathbf{q}'_{\perp}, t, t') &= 2 |F_G(\mathbf{q}')|^2 e^{-\int_{t'}^t \bar{\gamma}[(p_z + p'_z)/2](au) d\tau} \\ & \times \left[n(\mathbf{q}) \cos \left(\int_{t'}^t \frac{[\epsilon(p_z(\tau)) - \epsilon(p'_z(\tau)) - \hbar \omega_{\mathbf{q}'}] d\tau}{\hbar} \right) \right. \\ & \left. + [n(\mathbf{q}) + 1] \cos \left(\int_{t'}^t \frac{[\epsilon(p_z(\tau)) - \epsilon(p'_z(\tau)) + \hbar \omega_{\mathbf{q}'}] d\tau}{\hbar} \right) \right], \end{aligned} \quad (36)$$

$$\begin{aligned} \bar{\gamma}(p) &= \sum_{\mathbf{q}''} 2\pi\hbar |F_G(\mathbf{q}'')|^2 \{ [n(\mathbf{q}'') + 1] \delta(\epsilon(p) - \epsilon(p - \hbar q''_z)) \\ & \quad - \hbar\omega + n(\mathbf{q}'') \delta(\epsilon(p) - \epsilon(p + \hbar q''_z) + \hbar\omega) \}. \end{aligned} \quad (37)$$

We note that the Boltzmann out-scattering rate $\bar{\gamma}$ is formally obtained from γ by replacing the phonon coordinates $n_{\mathbf{q}''}$ by their expectation value $n(\mathbf{q}'')$.

V. PHYSICAL ASPECTS

A. Two models

We consider the derivation of the two models from a heuristic point of view. A basic step is the truncation of the GWF hierarchy at the first or the second off-diagonal level. A reasonable argument for such truncation is the assumption of a weak electron-phonon coupling. That is, F , multiplied by the corresponding momentum scale and the time scale β_t of the transitions between the GWF elements, must be small. An initially decoupled electron-phonon system is assumed, where all off-diagonal elements are zero. A typical Levinson transition links a diagonal element to a first off-diagonal element which is linked back to a diagonal element. Two transitions related to the left phonon basis are shown in Fig. 1. A single-phonon mode \mathbf{q}' is involved in both links. After the transition, the electron-phonon system returns back to the diagonal state. The assumption for a weak coupling means that only single events occur at a given time. Events where two or more transitions involving two or more phonon modes occur at the same time are highly improbable. Such events are neglected along with events involving higher off-diagonal elements in the path diagonal \rightarrow diagonal element.

As inferred by the integral form of Eq. (12), the duration of such transition is given by the time interval $t-t'$ in Eq. (13). The evolution of the system proceeds on a different time scale β_e which is larger than β_t . This time scale is relevant to the duration T of the measurement of the state of the system. The Levinson transport picture can be established if the system is mainly decoupled during the process of measurement; i.e., the cumulative time of all transitions is a very small part of the averaging time T : $\beta_e \gg \beta_t$. This is in accordance with the assumption (9) for an equilibrium phonon system (Bloch assumption), which associates a vast mechanism recovering the phonon equilibrium between the transitions.

A nice feature of the Levinson equation is that the classical limit of Eq. (13) recovers the Boltzmann equation. This feature leads to a model that explains the evolution in a wide time range in terms of Levinson transitions. In the long-time limit these transitions become the instantaneous Boltzmann scattering events. However, this model cannot be valid: A mechanism which keeps the transitions bounded in time is lacking in the Levinson equation. Indeed, the scattering function S , Eq. (13), is not vanishing for large transition times ($t-t'$) so that the time of a transition can become of order of the evolution time, $\beta_t \approx \beta_e$. From these considerations it is anticipated that the Levinson model can be relevant up to moderate evolution times.

The Barker-Ferry equation enters one level deeper in the hierarchy by incorporating the interaction of the FOD with the SOD elements. The main transitions are still of the Levinson type: The diagonal element n, n in Fig. 2 is linked to the diagonal element $n+1', n+1'$ via the FOD element $n+1', n$. Here the prime is for the mode \mathbf{q}' involved in the link. However, the FOD element is modified now by the coupling with the SOD elements as shown in the figure. The coupling involves a second mode \mathbf{q}'' and corresponds to instantaneous transitions from FOD to SOD elements and back. These transitions are integrated into the exponent of Eq. (36): To see this we compare Eq. (7) with Eq. (A3) and recall the equivalence of the latter with Eq. (A5) (with λ_1 set to zero). We note that the bounds of the time integral in the exponent correspond to the duration of the main transition, while the classical limit makes the interaction with the SOD elements instantaneous. All such SOD elements are accounted for by a sum over the second mode \mathbf{q}'' . The Barker-Ferry model already introduces a mechanism, which takes care of the duration of the transitions: the exponent effectively damps the long lasting correlations. However, in the long-time limit the model fails to recover the classical δ function, giving rise to a Lorentzian energy distribution instead.

These considerations suggest the existence of a time limit \mathcal{T} of validity of the two models. The correlations with the higher off-diagonal elements can no more be neglected after this time. An estimation of \mathcal{T} , which certainly depends on the physical parameters of the system, can be obtained by numerical experiments. A credibility guess for \mathcal{T} is the time when the behavior of the observables begins to become unphysical. As already noted, the Lorentzian gives rise to artificial carrier heating, so that the total energy of the system is one of the candidate observables. Is the carrier density also such an observable? An integration of Eq. (12) or (35) with

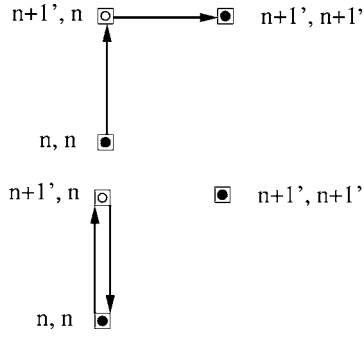


FIG. 1. Levinson transitions link diagonal with FOD elements. The FOD element is presented by the open circle, and n and n stand for the left and right phonon sets $\{n_q\}$ and $\{n_q\}$.

respect to p_z shows that the two models give rise to the continuity equation. Hence, if the initial condition is physically relevant, one cannot expect surprises in the evolution of the carrier density such as appearance of negative carrier concentrations. However, nothing can be set in advance for the evolution of the momentum density. While in the classical case the non-negative Boltzmann scattering rate guarantees a physical momentum distribution, the rates (13) and (36) allow negative values. Thus the behavior of the momentum density at longer evolution times could be another candidate for probing the validity of the models.

B. Phonon system

The appearance of the Boltzmann out-scattering rate $\bar{\gamma}$ in Eq. (37) can be established in two ways. One can follow the quite common approach of replacement of complicated functions by appropriate averages. As the phonons are assumed in equilibrium, the probability to find n_q phonons in mode \mathbf{q} is $P(n_q)$. By recalling the dependence of γ on $\{n_q\}$ it sufficient to average γ to obtain

$$\bar{\gamma} = \sum_{\{n_q\}} \prod_{\mathbf{q}} P_{eq}(n_q) \gamma. \quad (38)$$

Further on $\bar{\gamma}$ is replaced in the generalized equation (8) and the steps associated with Eqs.(9)–(11) are applied afterwards.

There is an alternative approach, which throws more insight in the assumptions hidden in Eq. (38). We adopt the treatment of the phonon system developed in Ref. 43 and accomplish the proof with the help of combinatorial considerations. In the generalized equation (8) we first expand $e^{-\int_t^t \gamma}$ into a series and truncate to a term K corresponding to a desired precision. Then we apply the trace operation together with the ansatz (9). Terms are obtained of the form

$$\sum_{\{n_q\}} n_{q_0} \sum_{q_1} n_{q_1} \sum_{q_2} (n_{q_2} + 1) \cdots P_{eq}(n_{q_0} + l) \prod_{q \neq q_0} P_{eq}(n_q) \times |F_G(\mathbf{q}_1)|^2 |F_G(\mathbf{q}_2)|^2 \cdots \delta_{q_1} \delta_{q_2} \cdots. \quad (39)$$

Here the sum of the trace runs over the natural numbers from zero to infinity for any mode. As shown below, we can take the average of any phonon mode \mathbf{q} independently on the rest of the modes in Eq.(39). That is, under a reasonable assump-

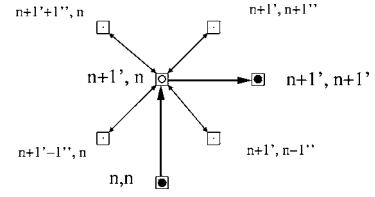


FIG. 2. The Barker-Ferry counterpart of the first Levinson transition shown on Fig. 1. Here $\pm 1''$ denotes an increase or decrease by unity of the phonons in mode \mathbf{q}'' in the left or right basis.

tion, with repeating modes of the form $n_q n_q \cdots P_{eq}(n_q)$ can be neglected. The first factor n_{q_0} corresponding to \mathbf{q}' in Eq. (8) is distributed according $P_{eq}(n_{q_0} + l)$, where l is ± 1 or 0 . With the help of Eq. (11) it is evaluated as $n(\mathbf{q}_0)$ or $n(\mathbf{q}_0) + 1$ and can be skipped in the further discussions. The modes $\mathbf{q}_1 \mathbf{q}_2 \cdots$ come from the product $\gamma \gamma \cdots$ in the expansion of the exponent. The phonons in these modes are distributed according $P_{eq}(n_q)$. After averaging, the equilibrium phonon numbers $n(\mathbf{q}_i)$ replace the corresponding phonon coordinates n_{q_i} in Eq. (39). These terms are summed to recover the exponent, which settles the appearance of $\bar{\gamma}$ in Eq. (36).

Now we show that, if the number of the modes in the plane normal to the wire is large enough, the trace can be taken by neglecting the terms with repeating modes in the product (39). The δ functions in γ affect only the z coordinates of the wave vectors as indicated by the index in $\delta_{q_{z1}}$. With this, Eq. (39) can be further decomposed into products with fixed combinations of z coordinates $q_{z1} q_{z2} \cdots q_{zk}$:

$$\sum_{n_{q_1} \cdots n_{q_k} = 0}^{\infty} \sum_{\mathbf{q}_{\perp 1}} n_{q_1} \cdots \sum_{\mathbf{q}_{\perp k}} n_{q_k} P_{eq}(n_{q_1}) \cdots P_{eq}(n_{q_k}) \times |F_G(\mathbf{q}_1)|^2 \cdots |F_G(\mathbf{q}_k)|^2.$$

We note that modes where F_G is zero (e.g., in the zeros of the electron state in the normal plane) can be skipped in the sum. We assume that the number of these modes is negligible compared to the number N of the modes in the normal plane (normal modes). Consider the product

$$\sum_{n_{q_1} \cdots n_{q_k} = 0}^{\infty} n_{q_1} \cdots n_{q_k} P_{eq}(n_{q_0}) P_{eq}(n_{q_1}) \cdots P_{eq}(n_{q_k}). \quad (40)$$

This expression is evaluated as

$$n(\mathbf{q}_1) \cdots n(\mathbf{q}_k), \quad \text{if } \mathbf{q}_1 \neq \mathbf{q}_2 \neq \cdots \neq \mathbf{q}_k, \quad (41)$$

or if some modes coincide to

$$n(\mathbf{q}_1) \cdots n^{(\alpha)}(\mathbf{q}_j) \cdots n^{(\beta)}(\mathbf{q}_m) \cdots n(\mathbf{q}_k), \quad (42)$$

$$n^{(\alpha)}(\mathbf{q}) = \sum_{n_q=0}^{\infty} n_q^\alpha P_{eq}(n_q).$$

Now let l be the infimum and m_k the supremum defined as

$$L = \inf_{\mathbf{q}} n(\mathbf{q}) |F_G(\mathbf{q})|^2$$

$$M_k = \sup_{\alpha\beta \cdots \mathbf{q}_0 \cdots \mathbf{q}_k} n(\mathbf{q}_1) \cdots n^{(\alpha)}(\mathbf{q}_j) \cdots n^{(\beta)}(\mathbf{q}_m) \cdots n(\mathbf{q}_k); \quad |F_G(\mathbf{q}_1)|^2 \cdots |F_G(\mathbf{q}_k)|^2.$$

These numbers exist due to the discrete character of the modes. Moreover, l is different from zero since the zeros of F_G are already skipped. We evaluate the relative contributions of the terms (42) to the sum (40). As the number of the terms (41) is $N(N-1)\cdots(N-k+1)$ (we assume the worst case scenario of equal z coordinates) this contribution is less than

$$\frac{M_k [N^k - N(N-1)\cdots(N-k+1)]}{L^k N(N-1)\cdots(N-k+1)}.$$

The latter tends to zero if N tends to infinity for any fixed $k \leq K$. It is concluded that if the number of the normal modes is very large we can keep only the terms (41). This result concerns also the Bloch assumption: An initially equilibrium phonon system can be considered as equilibrium at later times provided that the number of modes is large enough. In this case the assumption for a vast mechanism of phonon relaxation is no longer indispensable.

VI. RESULTS

The implemented numerical approach is a backward Monte Carlo method. The method has been developed and refined for both classical and quantum transport.^{25,39,44–50} The idea of the approach is to express the solution of the equation in a Neumann series and to evaluate the consecutive terms with the help of Markov chains. The latter are constructed by consecutive application of an *a priori* transition probability. The Markov chains begin from the fixed point and time where the value of the solution is to be determined. The chains “evolve” backward in time, which gives the name of the approach. In general the precision depends on the number of chains N as $N^{-1/2}$. High precision is obtained by increasing the number N , which is the expense of a corresponding increase of the computational time.

The approach is readily generalized for evaluation of functionals of the solution. In the indirect way the solution is computed at selected points which are used in the chosen quadrature for computation of the functional. In the direct way the functional is computed with the help of an initial probability used to select the initial points of the Markov chains.

A GaAs quantum wire with a square cross section of 10 nm is chosen for the simulations. The material parameters are taken from, Ref. 25; in particular, a single polar optical phonon having a constant energy $\hbar\omega$ is considered. The electric field is zero. The initial condition is a product of two Gaussian distributions of energy and space. The k_z^2 distribution corresponds to a generating laser pulse with an excess energy of about 150 meV. The z distribution is centered around the origin of the coordinate system. We first regard

the evolution of the wave vector (and similarly the energy) and the density distributions given by the integrals

$$f(k_z, t) = \int dz f_w(z, \hbar k_z, t), \quad n(z, t) = \int dp_z f_w(z, p_z, t).$$

Here it is assumed that the initial condition is normalized to unity. The behavior of the energy distribution at very low temperatures can be used as a test of the correctness of our approach: as the wire electrons remain in the ground state in the normal plane the peculiarities of the evolution in the wire must be the same as in the homogeneous case. We recall the major features of the homogeneous evolution.^{18,43} Semiclassical electrons can only emit phonons and lose energy equal to a multiple of the phonon energy $\hbar\omega$. They evolve according to an energy distribution, patterned by replicas of the initial condition shifted towards low energies.⁵² Such electrons cannot appear in the region above the initial distribution. Because of the lack of an energy-conserving δ function, the quantum solutions demonstrate two effects of a deviation from semiclassical behavior. The replicas are broadened and the broadening reduces with time. A finite density of electrons appears in the semiclassically forbidden region above the initial condition. The wire electrons show the same behavior. The function $f(k_z, t)$ is symmetric with respect to the origin, and thus $f(k_z > 0, t)$ is a representative for the behavior of the energy distribution. Figure 3 shows the initial condition and the well-broadened curve $f(|k_z|, t)$ at time $t = 50$ fs of the evolution. The presence of electrons above the initial condition is visible at around $k_z = 60 [\times 10^{-2}/\text{nm}]$. At such small times there is no difference between the solutions of the Levinson and Barker-Ferry models. The broadening begins to shrink with an increase of the time (Fig. 4); the first peak to the left of the initial condition is already formed after 150 fs of evolution, and the second one comes up. The distance between the initial and first peaks corresponds to a shift with the phonon energy; however the curve is still wider as compared to an exact replica. The 175-fs curve is obtained by a direct evaluation of the functional for the wave vector density. The curves at earlier times are computed indirectly via the Wigner function evaluated in 800×260 z and k_z mesh points. The points are regularly distributed in the simulation domain with steps of 1 nm and $0.5 [\times 10^{-2}/\text{nm}]$, respectively. With the increase of the evolution time the indirect way becomes more inexact. Figure 5 compares the 175-fs densities obtained by direct and indirect computations from the Levinson model. The indirect curve is already unphysical. The result is independent on how precisely the Wigner function is evaluated in the chosen points provided that the mesh is kept fixed. This feature is associated with the fact that with the increase of the evolution time the Wigner function (Fig. 6) becomes less smooth and thus an increased number of mesh points are needed for a precise evaluation of the corresponding functionals. The Barker-Ferry curve plotted with the solid line in Fig. 5 is obtained by the direct way. A comparison with the Levinson counterpart shows that the exponent has a pronounced effect on the wave vector distribution. It causes an effective retardation to the evolution process. The difference between the two models is

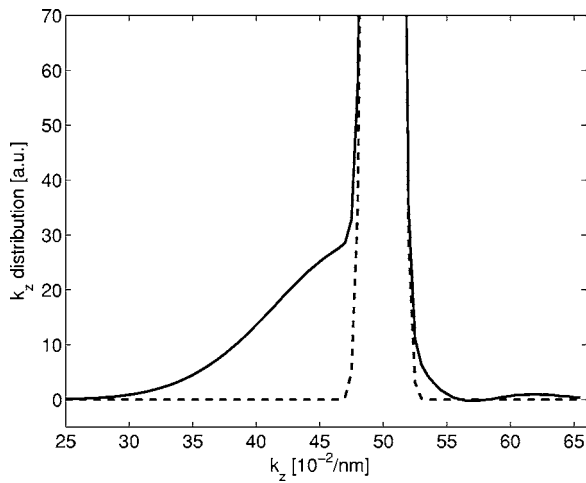


FIG. 3. Initial peak (dashed line) and the 50-fs wave vector density presented in a window of positive k_z .

expected to become more pronounced at larger times. Unfortunately the computational burden increases exponentially with the evolution time. Special numerical approaches are needed to achieve hundreds of femtoseconds, which is a task beyond the aims of this work.

Figure 7 shows the initial electron density (dashed line) centered around the origin. It splits into two peaks which move in the positive and negative directions of the wire. The 50-fs density is presented by the solid line. A comparison with the ballistic curve (dotted line) shows that at early times the spatial transport is mainly ballistic. An exception is the central part, already filled with electrons slowed down by the interaction with the phonons. The situation changes entirely with the increase of the time. Figure 8 compares the ballistic density with the densities obtained from the two models. The fronts of the ballistic peaks, placed above (below) 200 nm (-200 nm) are formed by the fastest classical electrons since processes of phonon absorption are suppressed at $T=0$ K. The quantum fronts are placed farther away from the origin.

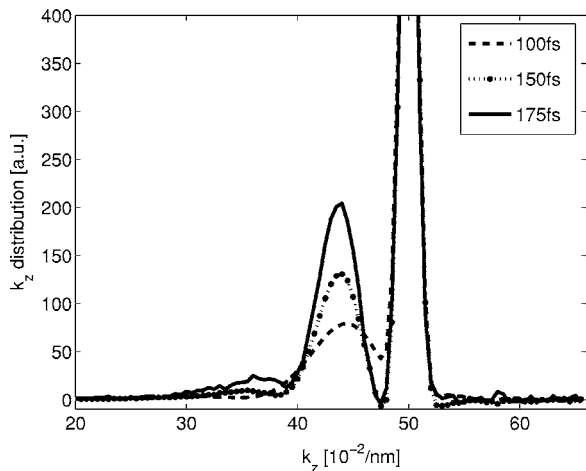


FIG. 4. Time evolution of the wave vector distribution obtained from the Levinson model. The 175-fs curve is obtained by direct evaluation of $f(k_z, t)$. The distributions at earlier times are computed indirectly, via the Wigner function.

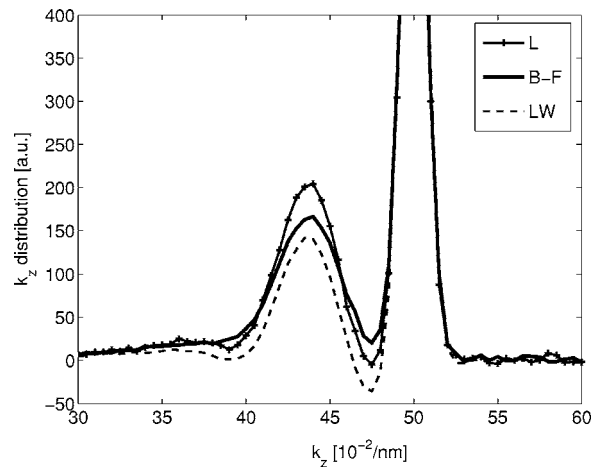


FIG. 5. The 175-fs wave vector distribution obtained from the Levinson model by direct (L) and indirect (LW) computations via the Wigner function. The difference between the two results is significant; the LW curve becomes negative in the valley between the peaks. The Barker-Ferry curve (solid line) is obtained by direct computations.

They are formed by electrons which gained velocity from the interactions: such electrons reside in the classically forbidden energy region and thus move faster. This picture is asserted by the distribution of the mean energy per particle,

$$e(z, t) = \int dk_z \epsilon(k_z) f(z, k_z, t) / n(z, t).$$

Figure 9 shows $e(z, t)$ for $t=175$ fs. The thin solid curve gives an initial reference for the energy range of the ballistic electrons. Outside the 200-nm region around the origin the quantum electrons are much hotter than the ballistic ones.

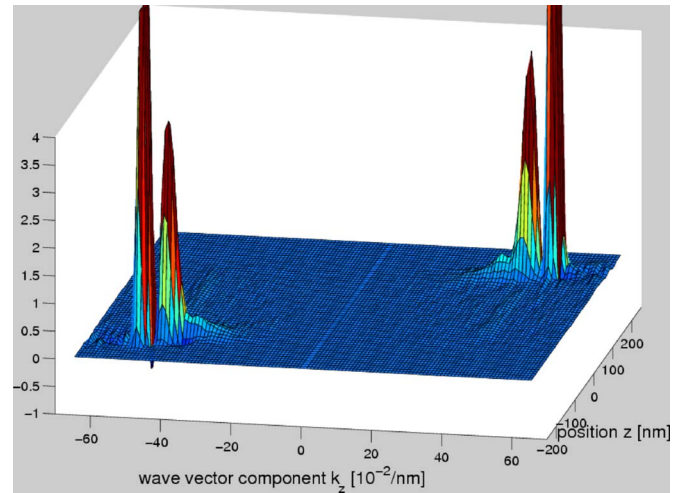


FIG. 6. (Color online) The Wigner function after 175 fs of evolution. The two main peaks are truncated for better resolution. The secondary peaks are formed by electrons which transferred part of their energy to the phonons. The classically forbidden regions are placed on the opposite side of the main peaks, in the nearest left and far right corners of the picture. The regions are populated with rapidly moving electrons.

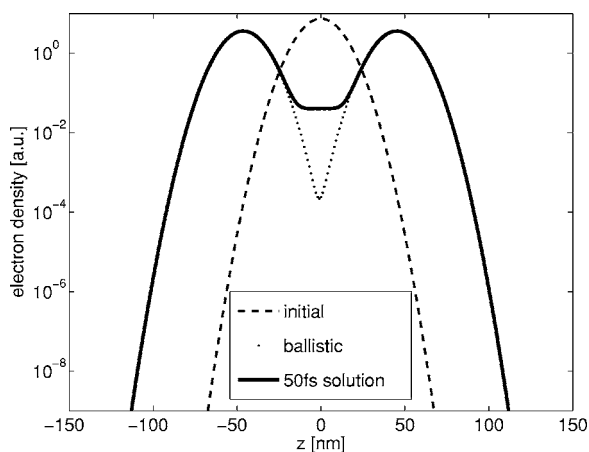


FIG. 7. Electron densities at time 0 and 50 fs. The ballistic curve (dotted line) coincides everywhere with the 50-fs solution apart from the central region. There reside electrons slowed down by the scattering events.

The difference of the energy distribution provided by the two models is already well pronounced in the central part. The Barker-Ferry curve is closer to the ballistic distribution which is in accordance with the delay in the evolution of the replicas caused by the exponential damping of the interaction durations.

VII. CONCLUSIONS

The generalized Wigner function provides a convenient approach for derivation of quantum-kinetic models of the electron-phonon interaction. The corresponding hierarchy of Wigner function elements can be truncated at different levels, giving rise to closed equations for the electron system. The inhomogeneous counterparts of the Levinson and Barker-Ferry equations, which describe the femtosecond evolution of local electron packets in a quantum wire, are

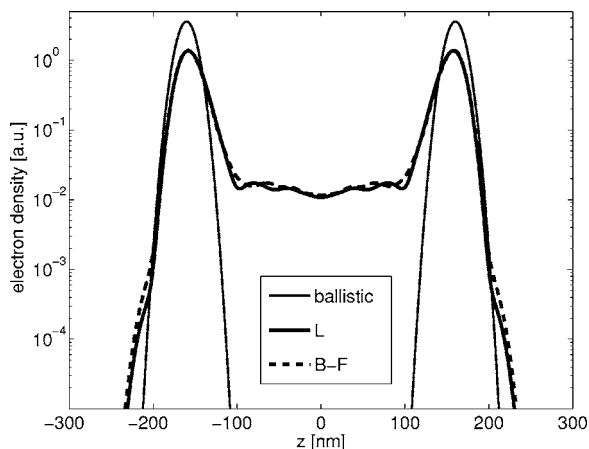


FIG. 8. Electron density after 175 fs evolution. The fastest classical electrons form the fronts of the two ballistic peaks (solid line) slightly above (below) 200 nm (−200 nm). The fastest quantum electrons of the Levinson (bold line) and Barker-Ferry (dashed line) models reach distances placed farther away from the origin.

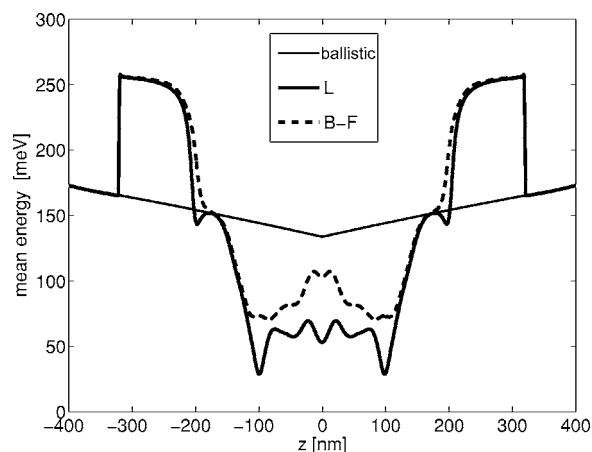


FIG. 9. Ballistic (solid line), Levinson (bold line), and Barker-Ferry (dashed line) distributions of the mean energy per particle at 175 fs.

derived. Basic to this are the hypotheses for an initially decoupled system, equilibrium phonons, and the Markov approximation. The physical aspects of the set of assumptions are discussed. In particular, it is argued that the relevance of both models is bounded at the long-time limit. The solutions of the equations are rich in quantum effects already in the case of zero electric field. Along with collisional broadening and retardation, an effect of ultrafast spatial transport is observed. This effect has been reported recently for the case of infinite electron lifetime.¹⁹ The solutions of the two models begin to differ after around 200 fs of evolution. The next few hundred femtoseconds are the most interesting time domain for analysis of the features of the two models. Unfortunately the numerical burden increases rapidly with the evolution time. Novel numerical approaches and implementation techniques, including GRID technologies, aiming to explore this time domain along with the effect of the electric field are currently under development.

ACKNOWLEDGMENT

This work has been partially supported by the Austrian Science Funds, FWF Project No. START Y247-N13.

APPENDIX A

The integral form of Eq. (2) is obtained with the help of the characteristics of the Liouville operator on the left, which are Newton's trajectories of the form

$$z(t') = z - \frac{1}{m} \int_{t'}^t p_z(\tau) d\tau, \quad p_z(t') = p_z - eE(t - t'). \tag{A1}$$

The particular trajectory is initialized at (z, p_z, t) . The equation includes explicitly the initial condition $f_0(z, p_z, \{n_q\}, \{n'_q\}, 0)$. The phonon coordinates of the particular terms remain the same in the integral form and the integro-differential counterpart. Referring to this correspondence we keep them implicit in the GWF elements:

$$\begin{aligned}
f_w(z, p_z, \cdot, t) &= f_0(z(0), p_z(0), \cdot, 0) e^{-i\hbar[\epsilon(\{n_{\mathbf{q}}\}) - \epsilon(\{n'_{\mathbf{q}}\})]t} \\
&+ \int_0^t dt' e^{-i\hbar[\epsilon(\{n_{\mathbf{q}}\}) - \epsilon(\{n'_{\mathbf{q}}\})](t-t')} \sum_{\mathbf{q}'} F(\mathbf{q}') \left\{ G(\mathbf{q}'_{\perp}) e^{iq'_z z(t')} \sqrt{n_{\mathbf{q}'}} + 1 f_w\left(z(t'), p_z(t') - \frac{\hbar q'_z}{2}, \cdot, t'\right) \right. \\
&- G^*(\mathbf{q}'_{\perp}) e^{-iq'_z z(t')} \sqrt{n_{\mathbf{q}'}} f_w\left(z, p_z(t') + \frac{\hbar q'_z}{2}, \cdot, t'\right) - G(\mathbf{q}'_{\perp}) e^{iq'_z z(t')} \sqrt{n_{\mathbf{q}'}} f_w\left(z, p_z(t') + \frac{\hbar q'_z}{2}, \cdot, t'\right) \\
&\left. + G^*(\mathbf{q}'_{\perp}) e^{-iq'_z z(t')} \sqrt{n_{\mathbf{q}'}} + 1 f_w\left(z(t'), p_z(t') - \frac{\hbar q'_z}{2}, \cdot, t'\right) \right\}. \tag{A2}
\end{aligned}$$

The integral form can be proved by taking the time derivative of Eq. (A2), which should lead us to Eq. (2). To see this we rewrite Eq. (A2) by keeping only the relevant variables:

$$\begin{aligned}
f(z, p_z, t) &= f(z(0), p_z(0), 0) e^{\lambda t} \int_0^t dt' K(z(t'), p_z(t')) e^{\lambda(t-t')} \\
&\times f(z(t'), p_z(t'), t'), \tag{A3}
\end{aligned}$$

which can be augmented to

$$\begin{aligned}
f(z(t''), p_z(t''), t'')|_{t''=t} &= f(z(0), p_z(0), 0) e^{\lambda t''}|_{t''=t} \\
&+ \int_0^{t''} dt' K(z(t'), p_z(t')) e^{\lambda(t''-t')} \\
&\times f(z(t'), p_z(t'), t')|_{t''=t}.
\end{aligned}$$

Written in this way, the equation reminds us that the time derivative is taken over the trajectory: first we differentiate with respect to t'' and set $t''=t$ in the final result. The left-hand side readily gives the Liouville operator \mathcal{L} acting on f , while the right-hand side gives $\lambda f(z, p_z, t) + K(z, p_z) f(z, p_z, t)$ [compare Eq. (2)]:

$$(\mathcal{L} - \lambda) f(z, p_z, t) = K(z, p_z) f(z, p_z, t). \tag{A4}$$

Equation (A3) can be formulated in an alternative way provided that $\lambda = \lambda_1 + \lambda_2$:

$$\begin{aligned}
f(z, p_z, t) &= f(z(0), p_z(0), 0) e^{\lambda_1 t} + \int_0^t dt' [K(z(t'), p_z(t')) \\
&+ \lambda_2] e^{\lambda_1(t-t')} f(z(t'), p_z(t'), t'). \tag{A5}
\end{aligned}$$

The equivalence between Eqs. (A3) and (A5) will be used in finding models which approximate Eq. (2). Note that Eqs. (A3) and (A5) continue to hold if λ is time dependent: then the argument of the exponents [of the form $\lambda(t-t_1)$, $t_1 = 0, t'$] must be replaced by $\int_{t_1}^t \lambda(\tau) d\tau$. We also note the equivalence between the expressions $p_z(t') + \hbar q_z$ and $(p_z + \hbar q_z)(t')$.

APPENDIX B

Denoting $f_w(\dots, t', \dots)$ shortly by $\phi(t')$ and introducing relative time variables $t_1 = t' - t''$, $\tau_1 = \tau - t''$ we rewrite the integral of interest I as follows:

$$\begin{aligned}
I &= \int_{t''}^t dt' e^{i \int_{t''}^{t'} [\Delta\epsilon(\tau) + \hbar\omega] d\tau / \hbar} \phi(t') \\
&= \int_0^{t-t''} dt_1 e^{i \int_0^{t_1} [\Delta\epsilon(\tau_1 + t'') + \hbar\omega] d\tau_1 / \hbar} \phi(t_1 + t'') \\
&= \int_0^{t-t''} dt_1 e^{(i/\hbar) \{ \Delta\epsilon(t'') + \hbar\omega + \hbar^2 q_z'' e E t_1 / 2m \} t_1} \phi(t_1 + t'').
\end{aligned}$$

The time integration in the last row has been performed with the help of the definition of the trajectory (A1) by using the explicit expression for $\Delta\epsilon$. Denote by α and β the scales of the energy and time, respectively. A dimensionless variable $t^\beta = t/\beta$ is introduced. We assume that α is a common scale for the electron and phonon energies and also for the term determined by the electric field, so that

$$\epsilon = \epsilon^\alpha \alpha, \quad \epsilon_{ph} = \hbar\omega = \epsilon_{ph}^\alpha \alpha, \quad \epsilon_E = \frac{\hbar^2 q_z e E \beta}{2m} = \epsilon_E^\alpha \alpha.$$

A new integration variable

$$x = \frac{t_1 \alpha}{\hbar} = \frac{t_1^\beta \beta \alpha}{\hbar} = \frac{t_1}{\hbar_\alpha} = \frac{t_1^\beta}{\hbar_{\alpha\beta}},$$

where $\hbar_\alpha = \hbar/\alpha$ and $\hbar_{\alpha\beta} = \hbar/(\alpha\beta)$, is introduced. Furthermore, the shortening $T = (t-t'')/\hbar_\alpha = (t-t'')^\beta/\hbar_{\alpha\beta}$ will be used. With the help of these variables the integral is rewritten as

$$I = \hbar_\alpha \int_0^T dx e^{i[\Delta\epsilon^\alpha + \epsilon_{ph}^\alpha + \epsilon_E^\alpha \hbar_{\alpha\beta}] x} \phi(\beta x \hbar_{\alpha\beta} + t'').$$

We assume that the energy and time scales are large enough to allow us to apply the limit $\hbar_{\alpha\beta} \rightarrow 0$. Then $T \rightarrow \infty$, while the term related to the electric field vanishes. The time integral in I becomes the Fourier transform of the step function $\theta(t)$ which is expressed with the help of generalized functions:

$$\begin{aligned}
I &= \hbar_\alpha \int_0^\infty dx e^{i[\Delta\epsilon^\alpha + \epsilon_{ph}^\alpha] x} \phi(t'') = \hbar \left(\pi \delta(\Delta\epsilon + \hbar\omega) \right. \\
&\left. + \text{VP} \frac{i}{\Delta\epsilon + \hbar\omega} \right) \phi(t'').
\end{aligned}$$

- ¹J. Schilp, T. Kuhn, and G. Mahler, *Phys. Rev. B* **50**, 5435 (1994).
- ²C. Furst, A. Leitenstorfer, A. Laubereau, and R. Zimmermann, *Phys. Rev. Lett.* **78**, 3733 (1997).
- ³M. Nedjalkov, H. Kosina, S. Selberherr, and I. Dimov, *VLSI Des.* **13**, 405 (2001).
- ⁴D. K. Ferry, A. M. Kriman, H. Hida, and S. Yamaguchi, *Phys. Rev. Lett.* **67**, 633 (1991).
- ⁵P. Bordone, D. Vasileska, and D. K. Ferry, *Phys. Rev. B* **53**, 3846 (1996).
- ⁶H. Hida, S. Yamaguchi, A. Kriman, and D. Ferry, *Semicond. Sci. Technol.* **7**, 8154 (1992).
- ⁷T. Kuhn and F. Rossi, *Phys. Rev. B* **46**, 7496 (1992).
- ⁸F. Rossi and T. Kuhn, *Rev. Mod. Phys.* **74**, 895 (2002).
- ⁹J. Barker, *Solid-State Electron.* **21**, 267 (1978).
- ¹⁰J. R. Barker and D. K. Ferry, *Phys. Rev. Lett.* **42**, 1779 (1979).
- ¹¹J. Barker and D. Ferry, *Solid-State Electron.* **23**, 519 (1980).
- ¹²W. Porod and D. Ferry, *Physica B & C* **134B**, 137 (1985).
- ¹³K. Thornber, *Solid-State Electron.* **21**, 259 (1978).
- ¹⁴M. V. Fischetti, *Phys. Rev. Lett.* **53**, 1755 (1984).
- ¹⁵P. Lipavski, F. S. Khan, F. Abdolsalami, and J. W. Wilkins, *Phys. Rev. B* **43**, 4885 (1991).
- ¹⁶D. Ferry, in *Physics of Nonlinear Transport in Semiconductors*, edited by D. Ferry, J. Barker, and C. Jacoboni (Plenum Press, New York, 1980), pp. 577–588.
- ¹⁷A. M. Kriman, N. C. Kluksdahl, and D. K. Ferry, *Phys. Rev. B* **36**, 5953 (1987).
- ¹⁸T. Gurov, M. Nedjalkov, P. A. Whitlock, H. Kosina, and S. Selberherr, *Physica B* **314**, 301 (2002).
- ¹⁹M. Herbst, M. Glanemann, V. M. Axt, and T. Kuhn, *Phys. Rev. B* **67**, 195305 (2003).
- ²⁰P. Lipavski, F. S. Khan, A. Kalvova, and J. W. Wilkins, *Phys. Rev. B* **43**, 6650 (1991).
- ²¹J. Rammer, *Rev. Mod. Phys.* **63**, 781 (1991).
- ²²A. V. Kuznetsov, *Phys. Rev. B* **44**, 8721 (1991).
- ²³I. Levinson, *Sov. Phys. JETP* **30**, 362 (1970).
- ²⁴M. Lindberg and S. W. Koch, *Phys. Rev. B* **38**, 3342 (1988).
- ²⁵M. Nedjalkov and I. Dimov, *Math. Comput. Simul.* **47**, 391 (1998).
- ²⁶J. Barker, in *Quantum Transport in Ultrasmall Devices*, edited by D. Ferry, H. Grubin, C. Jacoboni, and A. Jauho (Plenum Press, New York, 1995), p. 171.
- ²⁷L. Shifren, R. Akis, and D. Ferry, *Phys. Lett. A* **274**, 75 (2000).
- ²⁸M. Nedjalkov, H. Kosina, S. Selberherr, C. Ringhofer, and D. K. Ferry, *Phys. Rev. B* **70**, 115319 (2004).
- ²⁹M. Pascoli, P. Bordone, R. Brunetti, and C. Jacoboni, *Phys. Rev. B* **58**, 3503 (1998).
- ³⁰V. I. Tatarskii, *Sov. Phys. Usp.* **26**, 311 (1983).
- ³¹V. Spicka, B. Velicky, and A. Kalvova, *Physica E (Amsterdam)* **29**, 196 (2005).
- ³²F. Fromlet, P. Markowich, and C. Ringhofer, *VLSI Des.* **9**, 339 (1999).
- ³³J. B. Krieger, A. A. Kiselev, and G. I. Ifrate, *Phys. Rev. B* **72**, 195201 (2005).
- ³⁴N. Sano and K. Natori, *Phys. Rev. B* **54**, R8325 (1996).
- ³⁵N. Sano and T. Furuta, *Phys. Rev. B* **48**, 1426 (1993).
- ³⁶M. Nedjalkov, I. Dimov, and H. Haug, *Phys. Status Solidi B* **209**, 109 (1998).
- ³⁷L. Reggiani, P. Lugli, and A. Jauho, *J. Appl. Phys.* **64**, 3072 (1988).
- ³⁸L. Shifren and D. Ferry, *Phys. Lett. A* **306**, 332 (2003).
- ³⁹F. Rossi, C. Jacoboni, and M. Nedjalkov, *Semicond. Sci. Technol.* **9**, 934 (1994).
- ⁴⁰A. Bertoni, P. Bordone, R. Brunetti, and C. Jacoboni, *J. Phys.: Condens. Matter* **11**, 5999 (1999).
- ⁴¹C. Jacoboni and P. Bordone, *Rep. Prog. Phys.* **67**, 1033 (2004).
- ⁴²H. Haug and S. W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, 3rd ed. (World Scientific, Singapore, 1994).
- ⁴³R. Brunetti, C. Jacoboni, and F. Rossi, *Phys. Rev. B* **39**, 10781 (1989).
- ⁴⁴C. Jacoboni, P. Lugli, R. Brunetti, and L. Reggiani, *Superlattices Microstruct.* **2**, 209 (1986).
- ⁴⁵C. Jacoboni, P. Poli, and L. Rota, *Solid-State Electron.* **31**, 523 (1988).
- ⁴⁶P. Vitanov, M. Nedjalkov, C. Jacoboni, F. Rossi, and A. Abramo, in *Advances in Parallel Algorithms*, edited by Bl. Sendov and I. Dimov (IOS Press, Amsterdam, 1994), pp. 117–128.
- ⁴⁷H. Kosina, M. Nedjalkov, and S. Selberherr, in *Large Scale Scientific Computations 2003, LNCS 2907*, edited by I. Lirkov, S. Margenov, and P. Yalamov (Springer-Verlag, Berlin, 2004), pp. 170–177.
- ⁴⁸H. Kosina, M. Nedjalkov, and S. Selberherr, *J. Appl. Phys.* **93**, 3553 (2003).
- ⁴⁹T. Gurov and P. Whitlock, *Math. Comput. Simul.* **60**, 85 (2002).
- ⁵⁰C. Jacoboni and F. Rossi, in *Ultrashort Processes in Condensed Matter*, edited by W. Brown (Plenum Press, New York, 1993), pp. 287–335.
- ⁵¹M. A. Osman and D. K. Ferry, *Phys. Rev. B* **36**, 6018 (1987).
- ⁵²The existence of the phonon replicas can be contrasted with those found in semiclassical EMC simulations of ultrafast laser excitation (Ref. 51).