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1999 J. Phys.: Condens. Matter 11 5999

(http://iopscience.iop.org/0953-8984/11/31/308)

J. Phys.: Condens. Matter **11** (1999) 5999–6012. Printed in the UK PII: S0953-8984(99)01390-9

The Wigner function for electron transport in mesoscopic systems

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Received 29 January 1999, in final form 9 March 1999

Abstract. The Wigner-function approach to the quantum theory of electron transport in mesoscopic systems is reviewed. Delta-like or 'particle' contributions to the Wigner function are introduced that evolve in time along 'paths' formed by ballistic free flights separated by scattering processes like semiclassical particles. A Monte Carlo algorithm can be developed, based on such Wigner paths. Furthermore, a two-time Green function $G^<$ can be used to define a Wigner function where momentum and energy are treated as independent variables. The same Monte Carlo approach would then also yield the spectral function for the electron interacting with the phonon gas.

1. Introduction

The astonishing developments in semiconductor growth, characterization and processing technologies of the last two decades opened new exciting horizons in the field of experimental and theoretical semiconductor physics. The high degree of control of the material composition and of the sample geometry obtained with experimental techniques like molecular-beam epitaxy and electron-beam lithography allowed the production of low-dimensional structures, where transport and optical properties are strictly related to the particular dimensionalities of the systems. Furthermore, semiconductor structures are now available where the sample dimensions are comparable with the electron wavelength. They can sometimes be so small and so pure that, at low temperatures, carriers can cross the device under the action of an external field without experiencing any scattering event at all. Under these conditions the quantum nature of the charge carriers emerges, giving rise to new effects, not observed before for large samples.

The theoretical research in the field of semiconductor physics received an extraordinary impulse from the large amount of experimental data for these structures. New quantum theoretical approaches have been developed which go beyond the effective-mass theorem and the concept of the distribution function, and new effects predicted theoretically have been detected experimentally in real structures. The tremendous acceleration imparted by the increasing knowledge of the fundamental properties of low-dimensional and mesoscopic structures has already produced (and is still producing at increasing rates) technological applications.

The Wigner formulation of quantum mechanics [1] based on the concept of the Wigner function (WF) is particularly suitable for the study of quantum transport in mesoscopic systems since it allows one to describe quantum mechanical effects using a function defined in an $(\boldsymbol{r}, \boldsymbol{p})$ 'phase space', in analogy with what is done for classical systems. Furthermore, as we shall

0953-8984/99/315999+14$30.00

see, Wigner paths (WP) in this phase space can be defined which both provide a pictorial representation of the quantum evolution of the system of interest and constitute a useful tool for providing numerical solutions of the quantum equation describing the time evolution of the system of interest.

In this article a review of the authors' most recent advancements of the WF theory applied to the study of transport properties of mesoscopic systems is presented. In section 2 the definition of the WF together with some of its fundamental properties are summarized for the sake of completeness. In section 3 the theory is applied to coherent transport, i.e., to the case of transport in the absence of phase-breaking scattering. In section 4 the formulation of a general evolution equation for the WF of an electron gas in the presence of external/structural potentials and phonon scattering is presented, and the Neumann expansion of this equation is discussed with a view to using a perturbative approach to its solution. In section 5 the concept of Wigner paths is introduced and its use in a Monte Carlo-like solution of the WF evolution equation is discussed. In section 6 the two-time Wigner function is introduced as a theoretical tool for carrying information about both the carrier energy and momentum distributions, separately. In section 7 some conclusions are finally summarized.

2. The Wigner function

For a system formed by a single electron described by the density matrix operator ρ, the WF is defined as [1, 2]

$$f_W(\boldsymbol{r}, \boldsymbol{p}, t) = \int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \left\langle \boldsymbol{r} + \frac{\boldsymbol{s}}{2} \middle| \rho(t) \middle| \boldsymbol{r} - \frac{\boldsymbol{s}}{2} \right\rangle. \tag{1}$$

Here the normalization has been chosen in such a way that

$$\frac{1}{h^3} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{p}\; f_W(\boldsymbol{r}, \boldsymbol{p}, t) = 1. \tag{2}$$

In this way, if f_W is multiplied by the total number of electrons N in the system, then it should be comparable with the occupation number.

The WF is a real numerical function defined in the phase space $(\boldsymbol{r}, \boldsymbol{p})$ with many properties that resemble those of the classical distribution function. In particular, the mean value of the measure of a quantity described by the observable $\boldsymbol{A}$, averaged over the statistical ensemble, is given by

$$\langle \boldsymbol{A} \rangle = \frac{1}{h^3} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{p}\; A_W(\boldsymbol{r}, \boldsymbol{p}) f_W(\boldsymbol{r}, \boldsymbol{p}, t) \tag{3}$$

where

$$A_W(\boldsymbol{r}, \boldsymbol{p}) = \int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \left\langle \boldsymbol{r} + \frac{\boldsymbol{s}}{2} \middle| \boldsymbol{A} \middle| \boldsymbol{r} - \frac{\boldsymbol{s}}{2} \right\rangle. \tag{4}$$

It should be noted that in equation (3) the WF appears linearly: the WF is already quadratic in the wavefunction and already itself contains the interference information.

Furthermore,

$$\frac{1}{h^3} \int \mathrm{d}\boldsymbol{r}\; f_W(\boldsymbol{r}, \boldsymbol{p}, t) = \overline{|\Phi(\boldsymbol{p}, t)|^2} \tag{5}$$

$$\frac{1}{h^3} \int \mathrm{d}\boldsymbol{p}\; f_W(\boldsymbol{r}, \boldsymbol{p}, t) = \overline{|\Psi(\boldsymbol{r}, t)|^2} \tag{6}$$

where Φ and Ψ are the wavefunctions of the system in momentum space and real space respectively and the bar indicates the ensemble average.

The WF, however, is not a probability density, since it can assume negative values, as a consequence of phase information. It is often called a 'quantum distribution function'.

Furthermore, the WF can contain very rapid oscillations as a function of $\boldsymbol{r}$ and/or $\boldsymbol{p}$. These could be eliminated with a coarse graining of phase space, as is done with the classical distribution function (which would otherwise consist of infinite spikes where the particles are, separated by regions with null value). More often, an averaging of the WF with a bi-Gaussian weighting is performed, yielding the Husimi distribution [2] that assumes only non-negative values.

Finally, we recall that the WF can assume values different from zero in regions of space where the wavefunction is zero, and where, therefore, the particle cannot be found (e.g., inside an Aharonov–Bohm ring).

If the full system, formed by the electron and the phonon gas, is considered, a generalized WF can be defined, that includes the phonon states in the density matrix [3]:

$$f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)=\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\middle|\rho(t)\middle|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle \tag{7}$$

where n_q is the occupation number of the phonon mode $\boldsymbol{q}$. In order to recover the original electron WF, a trace over the phonon states must be taken. As we shall see in the following, however, as long as only electron variables are considered, a closed equation for the WF can easily be obtained. In contrast, when phonon variables are added, the trace over phonons of the resulting equation does not lead to a closed equation for the electron WF, since the trace operation does not commute with the electron–phonon interaction Hamiltonian. The usual hierarchy of equations would be obtained [4]. In the present scheme, the equation is perturbatively solved for the generalized WF and the trace over the phonons is taken not for the equation itself, but for the solution obtained.

3. Coherent evolution

We study in this section the quantum dynamical evolution of an electron system in the absence of phonon interaction. This is actually the case for very pure semiconductor structures at extremely low temperatures. Let us assume that the eigenvalues ε_n and the eigenvectors $|\varphi_n\rangle$ of the electron Hamiltonian can be determined. If the basis of Hamiltonian eigenstates is inserted in equation (1), the WF describing the coherent evolution of the system is obtained:

$$f_W(\boldsymbol{r},\boldsymbol{p},t)=\sum_{nm} f_{nm}(\boldsymbol{r},\boldsymbol{p})\mathrm{e}^{-(\mathrm{i}/\hbar)(\varepsilon_n-\varepsilon_m)(t-t_0)}\frac{1}{h^3}\int \mathrm{d}\boldsymbol{s}\int \mathrm{d}\boldsymbol{p}'\ f^*_{nm}(\boldsymbol{s},\boldsymbol{p}')f_W(\boldsymbol{s},\boldsymbol{p}',t_0) \tag{8}$$

where the coefficients f_{nm} are given by

$$f_{nm}(\boldsymbol{r},\boldsymbol{p})=\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\langle \boldsymbol{r}+\boldsymbol{s}/2|\varphi_n\rangle\langle\varphi_m|\boldsymbol{r}-\boldsymbol{s}/2\rangle. \tag{9}$$

They constitute a unitary transformation and connect the generalized WF to the density matrix $\rho(n,m,t)$ and vice versa. The integral equation in equation (8) is linear in the unknown function f_W. This property guarantees that, if the WF at $t=t_0$ is the sum of several contributions, then each of them will evolve according to equation (8), and the solution of the equation at any given time $t>t_0$ will be given by the sum of the single contributions evaluated at the same time. Even though the WF is real, interference between these contributions can still occur as a cancellation of positive and negative values. If the initial WF is considered

as the integral of δ-like contributions, each of them, in the absence of external forces, carries its value following a classical path. In fact, for the case of a basis set of plane waves, the coefficients in equation (9) are given by

$$f_{nn'}(\boldsymbol{r}, \boldsymbol{p}) = \mathrm{e}^{(\mathrm{i}/\hbar)(\boldsymbol{p}_n - \boldsymbol{p}_{n'})\cdot\boldsymbol{r}}\,\delta\left(\boldsymbol{p} - \frac{\boldsymbol{p}_n + \boldsymbol{p}_{n'}}{2}\right). \tag{10}$$

The ballistic evolution of an initial δ-like contribution to the WF, $\delta(\boldsymbol{r} - \boldsymbol{r}_0)\,\delta(\boldsymbol{p} - \boldsymbol{p}_0)$, is obtained from equation (8) after some straightforward calculations and turns out to be

$$\delta(\boldsymbol{r} - [\boldsymbol{r}_0 + \boldsymbol{p}/m(t - t_0)])\,\delta(\boldsymbol{p} - \boldsymbol{p}_0). \tag{11}$$

The above equation can be interpreted as follows: each δ-like contribution to the WF, in the absence of external forces, carries its value following a classical path. This property is well illustrated in figure 1, where the free evolution of the WF for a Gaussian 'minimum-uncertainty' wave packet is illustrated in two-dimensional projections onto the plane (z, p_z) at different times after the initial one. The WF also has a 'wave-packet' form which is 'deformed' in time due to the different paths followed by its 'δ-like' components: representative points in phase space corresponding to high momentum values move faster than low-momentum representative points [5].

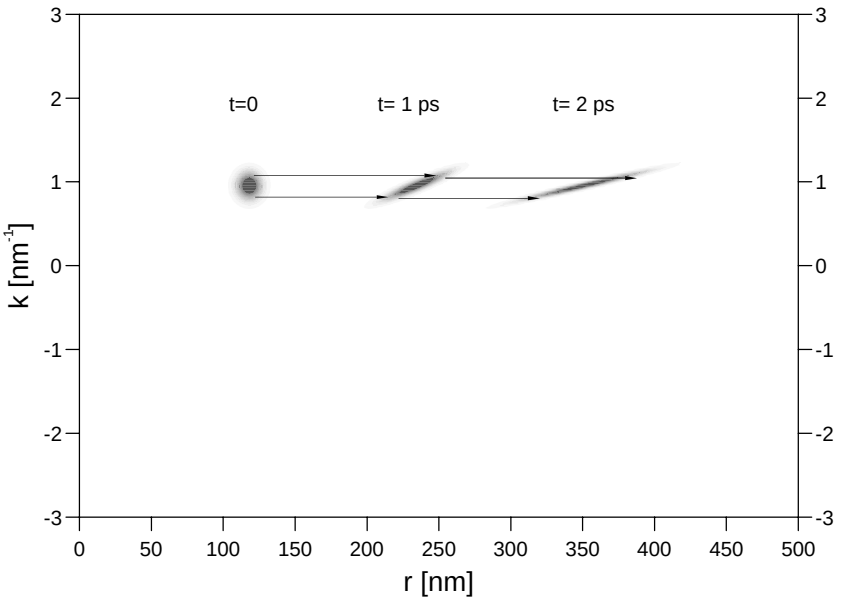

Figure 1. Free evolution in two-dimensional Wigner phase space of a WF for a wave packet. Each 'δ'-contribution of the WF follows a classical trajectory.

The results discussed above can be generalized to the case of electron Hamiltonians including a constant force or a harmonic potential. In these cases in fact, in the absence of collisions, the Wigner equation is identical to the Boltzmann equation for classical dynamics, as can be seen from equation (21), below. This concept of Wigner paths [6] will be discussed extensively in section 5 and has guided us in the development of the theoretical approach and of its numerical implementation.

4. The integro-differential equation

The general system that we are considering in this paper is formed by one electron (or, equivalently, many non-interacting electrons—ones that are not even interacting through the exclusion principle) subject to a constant and uniform accelerating field $\boldsymbol{E}$, to a structure potential $V(\boldsymbol{r})$ and to interaction with phonons. The Hamiltonian of the system is given by

$$\boldsymbol{H} = \boldsymbol{H}_0 + V(\boldsymbol{r}) + V_f(\boldsymbol{r}) + \boldsymbol{H}_p + \boldsymbol{H}_{e-p} \tag{12}$$

where

$$V_f(\boldsymbol{r}) = -e\boldsymbol{E}\cdot\boldsymbol{r}$$

and

$$\boldsymbol{H}_0 = -\frac{\hbar^2}{2m}\nabla_r^2$$
$$\boldsymbol{H}_p = \sum_q \boldsymbol{b}_q^\dagger \boldsymbol{b}_q \hbar\omega_q$$
$$\boldsymbol{H}_{e-p} = \sum_q \mathrm{i}\hbar F(\boldsymbol{q})(\boldsymbol{b}_q \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} - \boldsymbol{b}_q^\dagger \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}})$$

are, respectively, the free-electron term (with m-electron effective mass), the Hamiltonian for the free-phonon system and the electron–phonon interaction term. In the above expressions, $\boldsymbol{b}_q$ and $\boldsymbol{b}_q^\dagger$ are the annihilation and creation operators for the phonon mode $\boldsymbol{q}$, ω_q is the frequency of the phonon mode $\boldsymbol{q}$ and $F(\boldsymbol{q})$ is a function depending on the type of phonon scattering analysed.

If the time derivative of equation (1) is taken and the Liouville–von Neumann equation for the evolution of the density matrix is used, we find

$$\frac{\partial}{\partial t} f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q'\}, t) = \frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \left\langle \boldsymbol{r} + \frac{\boldsymbol{s}}{2}, \{n_q\} \middle| [\boldsymbol{H}, \rho(t)] \middle| \boldsymbol{r} - \frac{\boldsymbol{s}}{2}, \{n_q'\} \right\rangle. \tag{13}$$

In the following, the different terms of the Hamiltonian in equation (12) will be separately considered and developed.

4.1. The free-electron term

The term containing $\boldsymbol{H}_0$ gives rise to a term containing the space derivative of the distribution:

$$\begin{aligned}
&\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \left\langle \boldsymbol{r} + \frac{\boldsymbol{s}}{2}, \{n_q\} \middle| [\boldsymbol{H}_0, \rho(t)] \middle| \boldsymbol{r} - \frac{\boldsymbol{s}}{2}, \{n_q'\} \right\rangle \\
&\quad = -\frac{\hbar}{\mathrm{i}2m}\int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \Big\{ \nabla_r^2 \Psi(\boldsymbol{r} + \boldsymbol{s}/2, \{n_q\}, t)\Psi^*(\boldsymbol{r} - \boldsymbol{s}/2, \{n_q'\}, t) \\
&\qquad - \Psi(\boldsymbol{r} + \boldsymbol{s}/2, \{n_q\}, t)\nabla_r^2 \Psi^*(\boldsymbol{r} - \boldsymbol{s}/2, \{n_q'\}, t) \Big\} \\
&\quad = \frac{2}{m}\int \mathrm{d}\boldsymbol{s}\, \boldsymbol{p}\mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \cdot \Big\{ \boldsymbol{\nabla}_s \Psi(\boldsymbol{r} + \boldsymbol{s}/2, \{n_q\}, t)\, \Psi^*(\boldsymbol{r} - \boldsymbol{s}/2, \{n_q'\}, t) \\
&\qquad - \Psi(\boldsymbol{r} + \boldsymbol{s}/2, \{n_q\}, t)\, \boldsymbol{\nabla}_s \Psi^*(\boldsymbol{r} - \boldsymbol{s}/2, \{n_q'\}, t) \Big\} \\
&\quad = -\frac{\boldsymbol{p}}{m}\cdot\boldsymbol{\nabla}_r f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q'\}, t).
\end{aligned} \tag{14}$$

4.2. Potential scattering

The term due to the structure potential profile leads to [7]

$$\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\middle|[V(\boldsymbol{r}),\rho(t)]\middle|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle$$
$$=\int \mathrm{d}\boldsymbol{p}\ \mathcal{V}_W(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')f_W(\boldsymbol{r},\boldsymbol{p}',\{n_q\},\{n'_q\},t) \tag{15}$$

where the transfer function $\mathcal{V}_W$ is defined by

$$\mathcal{V}_W(\boldsymbol{r},\boldsymbol{p})=\frac{1}{h^3}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\frac{1}{\mathrm{i}\hbar}\left[V\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2}\right)-V\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2}\right)\right]. \tag{16}$$

4.3. The constant-field term

If the expression above for a general potential $V(\boldsymbol{r})$ is specialized to the case of a constant uniform electric field, such that $V(\boldsymbol{r})=-e\boldsymbol{E}\cdot\boldsymbol{r}$, then, after some calculation, one obtains

$$\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\middle|[V_f(\boldsymbol{r}),\rho(t)]\middle|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle$$
$$=\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}(e\boldsymbol{E}\cdot\boldsymbol{s})\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\},t\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\},t\right)$$
$$=e\int \mathrm{d}\boldsymbol{s}\ \boldsymbol{E}\cdot\boldsymbol{\nabla}_p\mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\},t\right)\Psi^*\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n'_q\},t\right)$$
$$=e\boldsymbol{E}\cdot\boldsymbol{\nabla}_p f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t). \tag{17}$$

Note that the same result would be obtained for a harmonic potential.

4.4. The free-phonon term

The term describing the free evolution of the phonon bath may be written as

$$\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\middle|[H_p,\rho(t)]\middle|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle$$
$$=\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\sum_{q'}\left\{\langle \boldsymbol{r}+\boldsymbol{s}/2,\{n_q\}|\boldsymbol{b}^\dagger_{q'}\boldsymbol{b}_{q'}\hbar\omega_{q'}|\Psi\rangle\langle\Psi|\boldsymbol{r}-\boldsymbol{s}/2,\{n'_q\}\rangle\right.$$
$$\left.-\langle \boldsymbol{r}+\boldsymbol{s}/2,\{n_q\}|\Psi\rangle\langle\Psi|\boldsymbol{b}^\dagger_{q'}\boldsymbol{b}_{q'}\hbar\omega_{q'}|\boldsymbol{r}-\boldsymbol{s}/2,\{n'_q\}\rangle\right\}$$
$$=\frac{1}{\mathrm{i}\hbar}(\mathcal{E}(\{n_q\})-\mathcal{E}(\{n'_q\}))f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) \tag{18}$$

where

$$\mathcal{E}(\{n_q\})=\sum_q n_q\hbar\omega_q \tag{19}$$

is the energy of the phonon state $\{n_q\}$.

4.5. Phonon scattering

The term due to electron–phonon interaction gives rise to four terms:

$$\begin{aligned}
&\frac{1}{\mathrm{i}\hbar}\int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\right|[H_{e-p},\rho(t)]\left|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle \\
&\quad = \int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}}\sum_{q'} F(\boldsymbol{q}') \\
&\qquad \times\left\{\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}-\boldsymbol{s}/2)}\sqrt{n_{q'}+1}\,\Psi\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n_1,\ldots,n_{q'}+1,\ldots\}\right)\Psi^*\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n'_q\}\right)\right. \\
&\qquad -\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}-\boldsymbol{s}/2)}\sqrt{n_{q'}}\,\Psi\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n_1,\ldots,n_{q'}-1,\ldots\}\right)\Psi^*\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n'_q\}\right) \\
&\qquad -\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}+\boldsymbol{s}/2)}\sqrt{n'_{q'}}\,\Psi\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n_q\}\right)\Psi^*\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n'_1,\ldots,n'_{q'}-1,\ldots\}\right) \\
&\qquad \left.+\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot(\boldsymbol{r}+\boldsymbol{s}/2)}\sqrt{n'_{q'}+1}\,\Psi\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n_q\}\right)\Psi^*\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n'_1,\ldots,n'_{q'}+1,\ldots\}\right)\right\} \\
&\quad = \sum_{q'} F(\boldsymbol{q}')\left\{\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\sqrt{n_{q'}+1}\,f_W\left(\boldsymbol{r},\boldsymbol{p}-\frac{\hbar\boldsymbol{q}'}{2},\{n_1,\ldots,n_{q'}+1,\ldots\},\{n'_q\},t\right)\right. \\
&\qquad -\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\sqrt{n_{q'}}\,f_W\left(\boldsymbol{r},\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2},\{n_1,\ldots,n_{q'}-1,\ldots\},\{n'_q\},t\right) \\
&\qquad -\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\sqrt{n'_{q'}}\,f_W\left(\boldsymbol{r},\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2},\{n_q\},\{n'_1,\ldots,n'_{q'}-1,\ldots\},t\right) \\
&\qquad \left.+\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\sqrt{n'_{q'}+1}\,f_W\left(\boldsymbol{r},\boldsymbol{p}-\frac{\hbar\boldsymbol{q}'}{2},\{n_q\},\{n'_1,\ldots,n'_{q'}+1,\ldots\},t\right)\right\}. \qquad (20)
\end{aligned}$$

The matrix element in the above equation contains two different sets of phonon occupation numbers $\{n_q\}$ and $\{n'_q\}$. Each term in the right-hand side of equation (20) represents a phonon interaction event (vertex) that changes only one set, increasing or decreasing the phonon occupation number of mode $\boldsymbol{q}'$ by unity and changing the electron momentum by $\hbar\boldsymbol{q}/2$.

4.6. The integral equation

Collecting the above results, the following equation is obtained:

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\boldsymbol{\nabla}_r-e\boldsymbol{E}\cdot\boldsymbol{\nabla}_p\right)f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) \\
&\quad = \frac{1}{\mathrm{i}\hbar}(\mathcal{E}(\{n_q\})-\mathcal{E}(\{n'_q\}))\,f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) \\
&\qquad + \int \mathrm{d}\boldsymbol{p}'\,\mathcal{V}_W(\boldsymbol{r},\boldsymbol{p}'-\boldsymbol{p})\,f_W(\boldsymbol{r},\boldsymbol{p}',\{n_q\},\{n'_q\},t)+\Xi(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)
\end{aligned} \qquad (21)$$

where $\Xi(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)$ represents the right-hand side of equation (20).

The left-hand side of equation (21) has the same form as the semiclassical Boltzmann equation. Thus path variables can be used in analogy with the Chambers formulation of

transport. Then, integrating over time, one obtains [8]

$$f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) = f_W\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t_0)+\frac{\boldsymbol{F}}{2m}(t-t_0)^2,\boldsymbol{p}-\boldsymbol{F}(t-t_0),\{n_q\},\{n'_q\},t_0\right)$$
$$\times \mathrm{e}^{-(\mathrm{i}/\hbar)(\mathcal{E}(\{n_q\})-\mathcal{E}(\{n'_q\}))(t-t_0)} + \int_{t_0}^{t} \mathrm{d}t'\, \mathrm{e}^{-(\mathrm{i}/\hbar)(\mathcal{E}(\{n_q\})-\mathcal{E}(\{n'_q\}))(t-t')}$$
$$\times \left\{ \int \mathrm{d}\boldsymbol{p}'\, \mathcal{V}_W\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t')+\frac{\boldsymbol{F}}{2m}(t-t')^2,\boldsymbol{p}'-\boldsymbol{p}+\boldsymbol{F}(t-t')\right)\right.$$
$$\times f_W\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t')+\frac{\boldsymbol{F}}{2m}(t-t')^2,\boldsymbol{p}',\{n_q\},\{n'_q\},t'\right)$$
$$\left. + \Xi\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t')+\frac{\boldsymbol{F}}{2m}(t-t')^2,\boldsymbol{p}-\boldsymbol{F}(t-t'),\{n_q\},\{n'_q\},t'\right)\right\} \tag{22}$$

with

$$\boldsymbol{F} = e\boldsymbol{E}. \tag{23}$$

The above equation shows that the value of the WF at a point $(\boldsymbol{r},\boldsymbol{p})$ at time t comes from three contributions:

(a) A ballistic term, equal to the WF's value at time t_0 on the trajectory of a classical particle, which is at $(\boldsymbol{r},\boldsymbol{p})$ at time t, and multiplied by a phase factor corresponding to the free evolution of the phonon bath.
(b) A term collecting, for each time t' and each transferred momentum $(\boldsymbol{p}-\boldsymbol{p}')$, contributions from the WF at points of phase space that, after a scattering by the potential, are on the 'right' classical trajectory that reaches $(\boldsymbol{r},\boldsymbol{p})$ at time t. This term is multiplied by the transfer function $\mathcal{V}_W$ acting as a weighting factor and by the free-phonon evolution phase factor.
(c) A term collecting for each time t' the four contributions of the electron–phonon interaction term. This last term will be discussed in more detail in the following.

5. Wigner paths, the phonon average and boundary conditions

5.1. Wigner paths

In section 3 we showed that, if neither potential nor phonon scattering is considered, a single δ-like contribution of the WF keeps its δ-character while evolving in time. Equation (22) shows that, taking into account phonon scattering, we may select a single scattering time t' and a single mode $\boldsymbol{q}'$ of the phonon interacting with the electron, and each δ-contribution still remains a δ. With the potential, we have to select a scattering time t' and a transferred momentum, and again a δ-like WF keeps its δ-character.

These considerations allow us to define a WP [6] as the path followed by a 'simulative particle' carrying a δ-contribution of the WF through the Wigner phase space. The concept of WP must not be confused with the concept of Wigner trajectories [9, 10] based on modified Hamilton equations. Only for potentials up to quadratic do WPs and Wigner trajectories coincide and coincide with classical trajectories [6].

Equation (22) may be iteratively substituted into itself giving a Neumann expansion describing the evolution of the WF by means of simulative particles following classical trajectories and experiencing two kinds of scattering:

(a) by a potential $V(\boldsymbol{r})$ that changes the particle's momentum from $\boldsymbol{p}'$ to $\boldsymbol{p}$;
(b) by an electron–phonon coupling that increases (decreases) by one the number of phonons in a phonon mode $\boldsymbol{q}$ of a single set $\{n_q\}$ and decreases (increases) a particle's momentum by $\overline{h}\boldsymbol{q}/2$.

The series obtained may be truncated to arbitrary order and solved by a Monte Carlo technique, sampling the integrals over the scattering times and the momentum transferred by the potential or phonons, in complete analogy to the 'weighted Monte Carlo' solution of the Boltzmann equation in its integral form [11].

As previously noted, we are interested in the evolution of a WF that is diagonal over phonon occupation numbers at the initial and final times. The requirement of initial diagonality is imposed by taking $f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n'_q\}, t_0) \neq 0$ only if $n_q = n'_q \ \forall \boldsymbol{q}$. To have a diagonal final WF, we simply write equation (22) for the specific $f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q\}, t)$. This choice implies that only terms containing a sequence of creation and annihilation operators that change in the same way (or do not change) the two sets of phonon occupation numbers are different from zero. As a consequence, only WPs with an even number of vertices involving a mode $\boldsymbol{q}$ are present.

As an example let us write out the unperturbed term and the first-order correction, in which no phonon interaction term is present:

$$f_W^0(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q\}, t) = f_W\left(\boldsymbol{r} + \frac{\boldsymbol{p}}{m}(t_0 - t) + \frac{\boldsymbol{F}}{2m}(t_0 - t)^2, \boldsymbol{p} + \boldsymbol{F}(t_0 - t), \{n_q\}, \{n_q\}, t_0\right) \tag{24}$$

$$\begin{aligned}\Delta^1 f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q\}, t) &= \int_{t_0}^{t} \mathrm{d}t' \int \mathrm{d}\boldsymbol{p}' \, \mathcal{V}_W\left(\boldsymbol{r} - \frac{\boldsymbol{p}}{m}(t - t') + \frac{\boldsymbol{F}}{2m}(t - t')^2, \boldsymbol{p}' - \boldsymbol{p} + \boldsymbol{F}(t - t')\right) \\ &\quad \times f_W^0\left(\boldsymbol{r} - \frac{\boldsymbol{p}}{m}(t - t') + \frac{\boldsymbol{F}}{2m}(t - t')^2, \boldsymbol{p}', \{n_q\}, \{n_q\}, t'\right).\end{aligned} \tag{25}$$

The expression for the second-order correction will contain each WP with two scattering events but, due to the diagonality requirement, only five terms will survive, representing five 'classes' of paths:

(1) paths with two potential scatterings,
(2) paths with a phonon absorption and a phonon emission at the second vertex,
(3) paths with a phonon absorption and a phonon emission at the first vertex,
(4) paths with phonon emissions at both vertices,
(5) paths with phonon absorptions at both vertices.

The paths associated with (3) and (4) are represented in the diagrams contained in figure 2(a). They correspond to the semiclassical paths where $\boldsymbol{q}/2$ is transferred to the electron at each vertex, while the dynamics between the two vertices is a ballistic evolution with the corresponding $\boldsymbol{p}$-value. If the process corresponds to a real transition, the second momentum transfer adds to the first one, so the total phonon momentum $\overline{h}\boldsymbol{q}$ is transferred to the electron. For virtual transitions at the second vertex of the interaction, half of the phonon momentum is given back to the phonon system and the electron recovers the original $\boldsymbol{p}$-value that it had at the beginning of the interaction. The path is anyway influenced by the virtual transitions, which are associated with the polaronic effect.

This interpretation can be extended to higher-order corrections (see, e.g., figure 2(b)). When time integrations are performed, each perturbative term contributes to the Wigner correction Δf_W by adding a sum over infinite paths like those represented in figure 2.

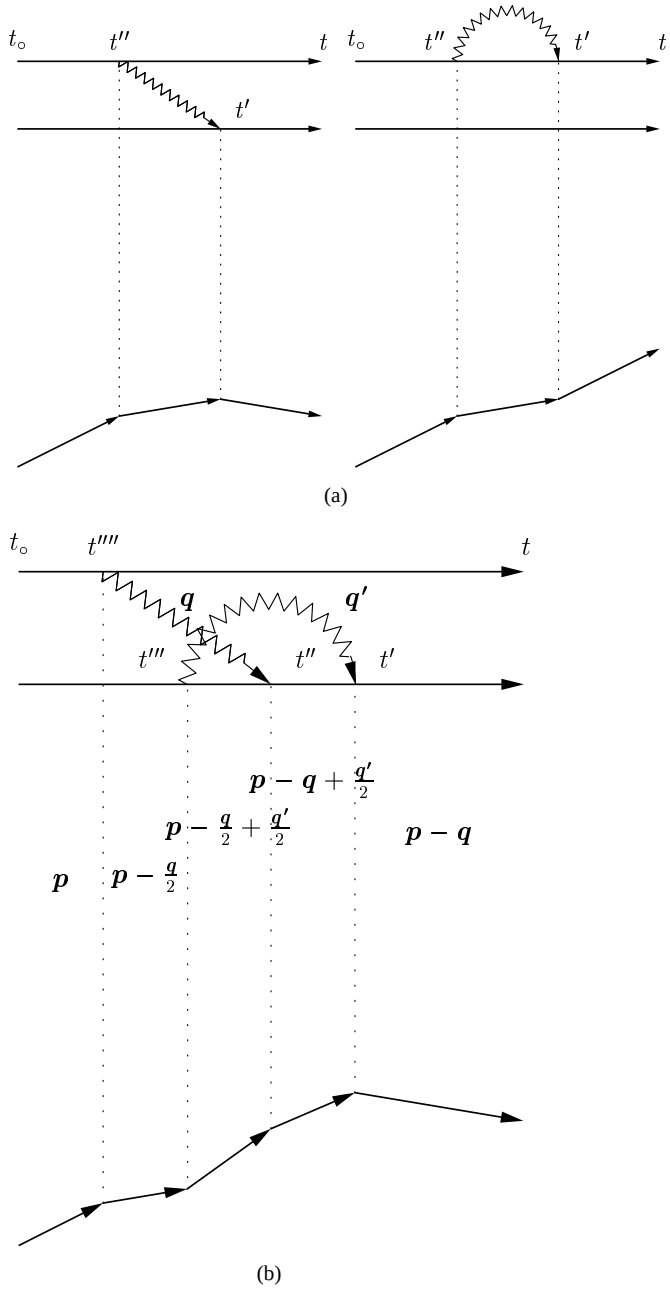

Figure 2. Examples of WPs. (a) A second-order contribution due to real (left) and virtual (right) emission of a phonon mode $\boldsymbol{q}$. (b) A fourth-order correction involving two phonon scatterings. The two time lines represent the action of the evolution operator on the two parts of the density matrix.

An integral over all possible WPs provides the evolution of the WF of the system of interest. A new computational approach to the solution of the Wigner quantum transport equation based on the generation of WPs is in currently being applied by the present authors.

5.2. The phonon average

A very important point not yet discussed here is how the trace over the phonon variables is taken. As stated above (section 2), such a trace operation is performed, in the present scheme, on the solution of the integral equation derived in the previous section. We assume, as an initial condition for our problem, a separate equilibrium density matrix, which is the product of an electron distribution function and the equilibrium phonon distribution, so the initial condition for the WF is

$$f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_{\boldsymbol{q}}\}, \{n_{\boldsymbol{q}}\}, t_0) = f_W^e(\boldsymbol{r}, \boldsymbol{p}, t_0) \prod_{\boldsymbol{q}} P_{eq}(n_{\boldsymbol{q}}) \tag{26}$$

where P_{eq} is the probability distribution for the occupation of the phonon mode $\boldsymbol{q}$. For the evaluation of contributions to the WF at time t which are diagonal in the phonon coordinates, each contribution to the scattering term in equation (22) contains a phonon mode twice and has factors like

$$\Delta f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_{\boldsymbol{q}}\}, \{n_{\boldsymbol{q}}\}, t) \propto n_1 \cdots (n_{\boldsymbol{q}'} + 1) \cdots f_W(\boldsymbol{r}, \boldsymbol{p}, \{n'_{\boldsymbol{q}}\}, \{n'_{\boldsymbol{q}}\}, t_0). \tag{27}$$

The generation of these terms is repeated a very large number of times for each $n_{\boldsymbol{q}}$. Then, if hot-phonon effects are ignored, we can have the following cases:

(a) For $\boldsymbol{q}$ not involved in a transition,

$$\sum_{\{n_{\boldsymbol{q}}\}} P_{eq}(n_{\boldsymbol{q}}) = 1. \tag{28}$$

(b) For real or virtual absorptions, taking into account how the phonon occupation numbers appear in equation (20),

$$\sum_{n_{\boldsymbol{q}}} (n_{\boldsymbol{q}} + 1) P_{eq}(n_{\boldsymbol{q}} + 1) = \langle n_{\boldsymbol{q}} \rangle \qquad \sum_{n_{\boldsymbol{q}}} n_{\boldsymbol{q}} P_{eq}(n_{\boldsymbol{q}}) = \langle n_{\boldsymbol{q}} \rangle . \tag{29}$$

Similarly, for real or virtual emissions,

$$\sum_{n_{\boldsymbol{q}}} n_{\boldsymbol{q}} P_{eq}(n_{\boldsymbol{q}} - 1) = \langle n_{\boldsymbol{q}} + 1 \rangle \qquad \sum_{n_{\boldsymbol{q}}} (n_{\boldsymbol{q}} + 1) P_{eq}(n_{\boldsymbol{q}}) = \langle n_{\boldsymbol{q}} + 1 \rangle . \tag{30}$$

In all cases we can eventually use the equilibrium Bose distribution for the evaluation of the scattering term without introducing any approximation to the electron–phonon coupling, but with the assumption that the phonon gas is kept at equilibrium.

5.3. Boundary conditions

The mathematical procedure described in the previous sections contains a formal integration over time of the differential equation obtained after the substitution of the path variables introduced. Let us now assume that the WF is known at time t_0 inside a closed region of phase space and at any time $t > t_0$ on its boundary. In such a case, instead of performing the time integration from t_0 to t, we can perform this integration from $\bar{t}$ to t, where $\bar{t} = t_0$ in the case where the 'ballistic path' that terminates at $(\boldsymbol{r}, \boldsymbol{p})$ at time t starts at t_0 inside the domain of interest; in the case where the 'ballistic path' crosses the boundary at a time $t_b > t_0$, we have $\bar{t} = t_b$. With this integration procedure and its iterative expansion, it can be seen that the WF in $\boldsymbol{r}$ at t is given by

(a) all paths that start inside the region of interest at time t_0 and end in $\boldsymbol{r}$ at time t after an arbitrary number of scattering events without exiting this region and
(b) all paths that enter the region of interest at any time after t_0 and again suffer any number of interactions inside [12].

This picture is again strictly analogous to the corresponding semiclassical transport picture.

It must be noted that the WF of the electron–phonon system must be known at the boundary of the system of interest. For example, if electrons are interacting with phonons while entering the region of interest, then this information must be contained in the boundary condition for the WF. If the boundary is located at a metallic contact, then we know that electron–electron interaction is very effective in destroying the phase correlation of the electron wavefunction that constitutes the difference between the WF and the semiclassical distribution function. In such a case it may be reasonable to use semiclassical boundary conditions [12]. In the general case it may be difficult to correctly account for electron–phonon interaction at the boundary and for the feedback of the device dynamics to the outside region near the boundary. These problems are not new. They have all been faced (and only partially solved) in semiclassical transport theory.

6. The two-time Wigner function

If the one-time density matrix in the definition of the WF is substituted for with the two-time density matrix (or the Green function $G^<$ [13]), and the proper Fourier transform is taken, the following WF is obtained:

$$f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},\omega,t) = \int \mathrm{d}\boldsymbol{s} \int \mathrm{d}\tau\ \mathrm{e}^{-\mathrm{i}((1/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}-\omega\tau)} \times \left\langle \boldsymbol{r}+\frac{\boldsymbol{s}}{2},\{n_q\}\middle|\rho(t+\tau/2,t-\tau/2)\middle|\boldsymbol{r}-\frac{\boldsymbol{s}}{2},\{n'_q\}\right\rangle \tag{31}$$

where $\boldsymbol{p}$ and ω are now to be considered as independent variables. Thus the WF contains information about both the momentum and energy of the electron, separately. The spectral density of the electron interacting with phonons and other agents would then be obtained. However, if the theory developed above is repeated for this new function, the same equation is obtained but with ω appearing as a parameter. The reason for this is that using a time-independent potential and including the phonons in the system leads to a time-independent Hamiltonian. In this case the energy is conserved and ω, which represents the total energy of the system, does not change as a consequence of the scattering events. Now one could think of the possibility of subtracting the potential energy at the point of the 'particle' and the energy of the phonon gas from the total energy to keep track of the electron kinetic and interaction energy. Unfortunately this is not possible, since during the scattering process (between two interaction vertices) the energy of the phonon gas is not well defined.

Alternatively it may be reasonable to consider the electron–phonon interaction as described by a time-dependent potential, as is usually done in the semiclassical theory of the interaction of radiation with matter. If electrons interact with an external potential $V(\boldsymbol{r},t)$ depending on time, the equation of motion for the WF turns out to be

$$\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\boldsymbol{\nabla}_r\right) f_W(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},\omega,t) = \int \mathrm{d}\boldsymbol{p}' \int \mathrm{d}\omega'\ \mathcal{V}_W(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}',\omega-\omega',t)\, f_W(\boldsymbol{r},\boldsymbol{p}',\omega,t) \tag{32}$$

where

$$\mathcal{V}_W(\boldsymbol{r},\boldsymbol{p},\omega,t) = \frac{1}{2\pi h^3}\int \mathrm{d}\boldsymbol{s}\ \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{p}\cdot\boldsymbol{s}} \int \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega\tau} \times \frac{1}{\mathrm{i}\hbar}\left[V\left(\boldsymbol{r}-\frac{\boldsymbol{s}}{2},t-\frac{\tau}{2}\right)-V\left(\boldsymbol{r}+\frac{\boldsymbol{s}}{2},t+\frac{\tau}{2}\right)\right]. \tag{33}$$

The suppression of the time dependence in V leads to the appearance of $\delta(\omega - \omega')$ on the right-hand side of equation (32), and equation (15) is recovered.

Let us consider now the phonons as an external classical field depending on time. In this case the electron–phonon interaction potential can be written as

$$V_{e-p}(t) = \sum_{q} (A_q \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\omega_0 t} - A_q^* \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\omega_0 t}) \tag{34}$$

where A_q is the amplitude of the phonon field corresponding to mode $\boldsymbol{q}$. The phonon distribution $\{n_q\}$ will then be reintroduced *a posteriori*. The equation of motion for the WF can then be written as

$$\begin{aligned}
\mathrm{i}\overline{h}\frac{\partial}{\partial t} f_W(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q'\}, \omega, t) = \sum_{q} \Bigg\{ & A_q \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\omega_0 t} f_W\left(\boldsymbol{r}, \boldsymbol{p} - \overline{h}\frac{\boldsymbol{q}}{2}, \omega - \frac{\omega_0}{2}, t\right) \\
& - A_q^* \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\omega_0 t} f_W\left(\boldsymbol{r}, \boldsymbol{p} + \overline{h}\frac{\boldsymbol{q}}{2}, \omega + \frac{\omega_0}{2}, t\right) \\
& - A_q \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{-\mathrm{i}\omega_0 t} f_W\left(\boldsymbol{r}, \boldsymbol{p} + \overline{h}\frac{\boldsymbol{q}}{2}, \omega + \frac{\omega_0}{2}, t\right) \\
& + A_q^* \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\omega_0 t} f_W\left(\boldsymbol{r}, \boldsymbol{p} - \overline{h}\frac{\boldsymbol{q}}{2}, \omega - \frac{\omega_0}{2}, t\right) \Bigg\}.
\end{aligned} \tag{35}$$

It should be noticed that this result corresponds to the one obtained previously, where the inclusion of the energy dependence is accounted for by adding (emission) or subtracting (absorption) half of the phonon energy at each interaction vertex, similarly to what must be done for the momentum transfer.

The path simulation approach described above for the traditional one-time WF can be followed also for the WF that carries separate information for electron energy and momentum. The initial/boundary condition must assume given values for $\boldsymbol{p}$ and ω (e.g. that of free particles: $\overline{h}\omega = \boldsymbol{p}^2/(2m) + V(\boldsymbol{r}) - e\boldsymbol{E}\cdot\boldsymbol{r}$). Then at each phonon vertex, half of the phonon energy must be transferred to (or from) the electron. At the final time t, the electron energy $\overline{h}\omega$ (containing the kinetic and interaction energy) is obtained by subtracting from $\overline{h}\omega$ the potential energy of the final position of the particle.

7. Conclusions

In the present paper we have presented a survey of the research performed by the authors in the field of the theory of quantum transport of electrons in mesoscopic systems. The traditional WF is extended to include phonons. The resulting integro-differential equation can be solved iteratively, with given initial and/or boundary conditions, and the trace over phonons can be taken for the solution obtained. Such a solution can be obtained as a sum of contributions, each due to a 'particle' path, formed by ballistic fragments described by classical dynamics (of free electrons or of electrons subject to a constant, uniform electric field), separated by interaction vertices due to electron–phonon or potential interaction. The absorption (or emission) of a phonon corresponds to two interaction vertices, each of which transfers half of the phonon momentum to the electron.

Between the two vertices of a phonon process, an applied field modifies the electron path (the intracollisional field effect) or other vertices may be present (multiple collisions). Energy conservation would be ensured by sufficient interference between all possible trajectories, but this interference is made incomplete by the occurrence of other scattering processes (collisional broadening).

The theory has also been extended to consider a two-time density matrix (or $G^<$ Green function) that leads to the definition of a WF that depends on the momentum and energy of the interacting electron, separately. The path description of the WF dynamics remains also in this case, and at each vertex half of the phonon energy is transferred to (or taken by) the electron.

A Monte Carlo approach to the evaluation of the WF of electrons in mesoscopic systems, very similar to the traditional Monte Carlo approach to semiclassical transport, can then be developed based on the WF paths discussed in this paper. If the two-time approach is assumed, a Monte Carlo derivation of the spectral density of electrons interacting with phonons would be obtainable.

Acknowledgment

This work was partially supported by ONR (Contract No N00014-98-1-0777).

References

[1] Wigner E 1932 *Phys. Rev.* **40** 749
[2] Hillery M, O'Connell R F, Scully M O and Wigner E P 1984 *Phys. Rep.* **106** 121
[3] Rossi F, Jacoboni C and Nedjalkov M 1994 *Semicond. Sci. Technol.* **9** 934
[4] Rickayzen G 1980 *Green Functions and Condensed Matter* (London: Academic)
[5] Brunetti R and Jacoboni C 1998 *Phys. Rev.* B **57** 1723
[6] Pascoli M, Bordone P, Brunetti R and Jacoboni C 1998 *Phys. Rev.* B **58** 3503
[7] Frensley W R 1990 *Rev. Mod. Phys.* **62** 745
[8] Rees H D 1972 *J. Phys. C: Solid State Phys.* **5** 64
[9] Lee H-W and Scully M 1983 *Found. Phys.* **13** 61
[10] Sala R, Brouard S and Muga J G 1993 *J. Chem. Phys.* **99** 2708
[11] Rossi F, Poli P and Jacoboni C 1992 *Semicond. Sci. Technol.* **7** 1017
[12] Bordone P, Pascoli M, Brunetti R, Bertoni A, Jacoboni C and Abramo A 1999 *Phys. Rev.* B **59** 3060
[13] Kadanoff L P and Baym G 1989 *Quantum Statistical Mechanics* (New York: Addison-Wesley)