INSTITUTE OF PHYSICS PUBLISHING SEMICONDUCTOR SCIENCE AND TECHNOLOGY
Semicond. Sci. Technol. **19** (2004) S226–S228 PII: S0268-1242(04)72081-7

A quasi-particle model of the electron–Wigner potential interaction

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Received 28 July 2003
Published 8 March 2004
Online at stacks.iop.org/SST/19/S226 (DOI: 10.1088/0268-1242/19/4/076)

Abstract
The Wigner equation was used for the calculation of carrier transport in mesoscopic devices. The carrier transport has a coherent part determined by the Wigner potential V_w and a dissipative part accounting for the interaction with phonons. Models have been developed which solve the equation by using quasi-particles evolving over pieces of classical Newton trajectories. In a backward evolution approach [1], the interaction with the Wigner potential is interpreted as a scattering process. The quantum information is carried by the particle weight. In the ensemble model proposed in [2], the quantum information from V_w is included by the particle affinity. Both weight and affinity are artificial numerical quantities. We propose a model which interprets the Wigner equation with a Boltzmann scattering term as a Boltzmann equation with a generation term. The quantum information is carried by the sign of the quasi-particles. In all other aspects quasi-particles behave as classical particles. The sign has a physical meaning since particles of opposite sign can annihilate. The model ensures a seamless transition between classical and quantum regions. Negative values of the Wigner function are explained in a direct way.

1. Introduction

Models which explain quantum phenomena in classical terms provide a convenient basis for the understanding and modelling of charge transport in mesoscopic structures. A useful formalism for the development of such models is provided by the Wigner function approach, which combines a rigorous quantum-kinetic picture with the classical concepts for phase space and open system boundary conditions.

Without loss of generality we introduce the model for the case of stationary transport in a one-dimensional device. The real space coordinate x of the device is bounded between two contact points 0 and L. The complete three-dimensional space of wave vectors $\mathbf{k} = (k_x, k_y, k_z)$ is considered.

$$\frac{\hbar k_x}{m}\frac{\partial}{\partial x} f_w(x,\mathbf{k}) = \int \mathrm{d}k'_x V_w(x, k'_x - k_x) f_w(x,\mathbf{k}) + \int \mathrm{d}\mathbf{k}' f_w(x,\mathbf{k}') S(\mathbf{k}',\mathbf{k}) - f_w(x,\mathbf{k})\lambda(\mathbf{k}) \tag{1}$$

where S denotes the phonon scattering rate and $\lambda(\mathbf{k}) = \int S(\mathbf{k},\mathbf{k}')\,\mathrm{d}\mathbf{k}'$ the total scattering rate. The Wigner potential is defined by the Fourier transform:

$$V_w(x,k_x) = \int \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}k_x s}\frac{1}{\mathrm{i}2\pi\hbar}\left(V\left(x-\frac{s}{2}\right) - V\left(x+\frac{s}{2}\right)\right) \tag{2}$$

where $V(x)$ is the device potential. Open system boundary conditions are provided by classical equilibrium functions $f_b(x_b,\mathbf{k})$, $b = 1, 2$ corresponding to the two reservoirs [3].

The characteristics of the Liouville operator are Newton trajectories which have a simple form for the chosen formulation (1): $x(t) = x + \frac{\hbar}{m}k_x t$, $\mathbf{k}(t) = \mathbf{k}$. An alternative formulation is obtained if the classical force term is separated from V_w and assigned to the Liouville operator on the left-hand side of (1) [4].

The Wigner function f_w is used to obtain all statistical averages of interest

$$\langle A\rangle = \int \mathrm{d}x \int \mathrm{d}\mathbf{k} f(x,\mathbf{k}) A(x,\mathbf{k}) \tag{3}$$

such as carrier density, velocity and current.

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2. Physical averages

A physical average $\langle A\rangle$ can be expressed in an alternative way to (3):

$$\langle A\rangle = \sum_{b=1,2}\int_{K_+(x_b)} \mathrm{d}\mathbf{k}_b \int_0^\infty \mathrm{d}t_0 |v_x(\mathbf{k}_b)| f_b(x_b,\mathbf{k}_b) \times \exp\left(-\int_0^{t_0}\mu(x_b(y),\mathbf{k}_b)\,\mathrm{d}y\right) g(x_b(t_0),\mathbf{k}_b). \tag{4}$$

This equation is obtained by a method described in [5] for the case of a classical distribution function. $K_+(x_b)$ is the part of the wave vector space with inward directed x-velocities. The function g is the solution of the adjoint integral equation of (1):

$$g(x,\mathbf{k}) = \int_0^\infty \mathrm{d}t \int \mathrm{d}\mathbf{k}'\Gamma(x,\mathbf{k}',\mathbf{k}) \times \exp\left(-\int_0^t \mu(x(y),\mathbf{k}')\,\mathrm{d}y\right)\theta_D(x) g(x(t),\mathbf{k}') + A(x,\mathbf{k}) \tag{5}$$

$$\Gamma(x,\mathbf{k}',\mathbf{k}) = S(\mathbf{k},\mathbf{k}') + \gamma(x)\delta(\mathbf{k}'-\mathbf{k}) + \left(V_w^+(x,k_x-k_x') - V_w^+(x,k_x'-k_x)\right)\delta(\mathbf{k}'_{yz}-\mathbf{k}_{yz}) \tag{6}$$

V_w^+ is a positive function defined as $V_w^+ = \max(V_w,0)$. The antisymmetry of V_w has been used in (6). The function $\gamma(x) = \int V_w^+(x,k_x)\,\mathrm{d}k_x$ is interpreted as the out-scattering rate of the Wigner potential in strict analogy with the phonon out-scattering rate λ [6]. Finally $\mu(x,\mathbf{k}) = \lambda(\mathbf{k}) + \gamma(x)$. The indicator of the device domain $\theta_D(x)$ is unity if $0 \leqslant x \leqslant L$ and zero otherwise. Using (4), physical averages can be directly obtained from the boundary conditions and the solution of the adjoint equation. The Neumann series of (5) replaced in (4) gives rise to a series expansion of the physical average $\langle A\rangle$. The expansion is analysed in terms of conditional probability densities. According to the theory of the numerical Monte Carlo method, conditional probability densities can be used to construct numerical trajectories. These can be interpreted as trajectories of quasi-particles which evolve in the phase space as Boltzmann-like particles.

3. Quasi-particle model

The strict analogy of (4) with its classical counterpart [5] allows a classical picture to be introduced where particles are injected from the contacts with a velocity-weighted equilibrium distribution. The state of an injected particle provides the initial point for a numerical trajectory. The transition probability for trajectory construction is given by the kernel in (5), which we rewrite as

$$K(x,\mathbf{k}',\mathbf{k},t) = \mu(x,\mathbf{k})\,\exp\left(-\int_0^t \mu(x(y),\mathbf{k}')\,\mathrm{d}y\right) \times \frac{\Gamma(x(t),\mathbf{k}',\mathbf{k})}{\mu(x,\mathbf{k})}\theta_D(x(t)). \tag{7}$$

The kernel describes a transition between an initial state $(x,\mathbf{k})$ and a final state $(x(t),\mathbf{k}')$. It is multiplied and divided by μ to obtain the probability density

$$p_t(t,x,\mathbf{k}) = \mu(x(t),\mathbf{k})\exp\left(-\int_0^t \mu(x(y),\mathbf{k})\,\mathrm{d}y\right).$$

p_t generates a value of t associated with the free flight time of a particle which drifts over a piece of a Newton trajectory between the initial state $(x,\mathbf{k})$ at time 0 and the final state $(x(t),\mathbf{k})$. This state is used in the remaining term $\Gamma(x(t),\mathbf{k}',\mathbf{k})/\mu(x(t),\mathbf{k})$ to select the value for $\mathbf{k}'$,

$$\frac{\Gamma(x,\mathbf{k}',\mathbf{k})}{\mu(x,\mathbf{k})} = p_1(x,\mathbf{k})\left\{\frac{S(\mathbf{k},\mathbf{k}')}{\lambda(\mathbf{k})}\right\} + (1-p_1(x,\mathbf{k})) \times \left(\left\{\frac{V_w^+(x,k_x-k_x')}{\gamma(x)}\right\} - \left\{\frac{V_w^+(x,k_x'-k_x)}{\gamma(x)}\right\} + \{\delta(k_x-k_x')\}\right)\delta(\mathbf{k}_{yz}-\mathbf{k}'_{yz})$$

where

$$p_1(x,\mathbf{k}) = \frac{\lambda(\mathbf{k})}{\mu(x,\mathbf{k})} \qquad 1-p_1(x,\mathbf{k}) = \frac{\gamma(x)}{\mu(x,\mathbf{k}).} \tag{8}$$

Normalized probability distributions are enclosed in curly brackets. p_1 is the probability for $\mathbf{k}'$ to be selected from the distribution S/λ. The case corresponds to a classical scattering event, where the particle changes its wave vector from $\mathbf{k}$ to $\mathbf{k}'$.

The alternative event occurring with probability $1-p_1$ corresponds to interaction with the Wigner potential. In this case, three normalized probability density functions have to be considered: the delta function $\delta(k_x-k_x')$ describes self-scattering, showing that the state $(x(t),\mathbf{k})$ is not changed by this interaction. In addition two new states $(x(t),k_x-q,\mathbf{k}_{yz})$ and $(x(t),k_x+q,\mathbf{k}_{yz})$ are created, which are interpreted as two particles. The momentum transfer q is generated from the density $V_w^+(x(t),q)/\gamma(x(t))$. At this point we associate with each particle a sign. The first particle bears the sign of the initial particle, the second one the opposite sign because of the minus in front of the corresponding term in (6). The sign of the particles is taken into account in the calculation of the sample mean. Finally, the contribution of a particle becomes zero only when the θ_D function in (7) becomes zero, which happens when the particle leaves the device.

The following picture is associated with the transport process. Quasi-particles are injected into the device from the boundaries and are subject to drift and scattering events, caused by the electron–phonon interaction. Particles have Boltzmann-like behaviour independently of their sign. The interaction with the Wigner potential occurs during the free flights, when pairs of positive and negative particles are generated according to the rules described. The picture corresponds to a Boltzmann equation with a generation term.

The sign of the particles is taken into account in the computation of the physical averages. A positive and a negative particle which meet in a given phase space point have a common probabilistic future. Such particles give opposite contributions to any statistical average. Hence particles with different signs annihilate when they meet in phase space.

The Wigner picture of quantum transport can be explained by the processes of generation and annihilation of positive and negative particles.

A useful property of the model is the seamless transition between classical and quantum domains. Such domains are determined by the values of the two out-scattering rates γ and λ. If $\lambda \gg \gamma$, the scattering with phonons dominates and the

transport is classical. In the opposite case, the interaction with phonons is rarely selected. Such conditions correspond to coherent transport when only pairs of particles are generated.

The model has been introduced for the case of stationary transport determined by the boundary conditions. A generalization to evolution problems determined by initial conditions is straightforward.

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