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Modeling of quantum transport in open systems

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Chapter 1

Introduction

The increasing usage of electronic devices based on charge transport in semiconductors confirms the fundamental role played by semiclassical- as well as quantum-transport theories. In fact, a large number of novel materials and devices are continuously designed and tested using various charge-transport models, and their applications fall in a lot of different fields, e.g., computer, medical, or biological science. apart from its applications, transport theory offers a unique opportunity to test very basic physical phenomena; typical examples are the discover of "Quantum Hall Effect" [1] or the surprising results obtained in "quantum interference devices" [2]. In the last two decades, as semiconductor technology has continued to pursue the down scaling of device dimensions into the submicron (less than 10000 Å) and ultrasubmicron (less than 1000 Å) regions, many new and interesting questions have emerged concerning the physics of small dimensions [3], specifically with regard to the need for a quantum development of transport in solid-state materials. Semiconductor transport in the ultrasubmicron region approaches the so-called quantum limit; In such a regime it is necessary to face new basic problems, not present in the semiclassical scenario. For example, the "measurement" and/or the "open system" problems may play a dominant role in the study of semiconductor-based quantum devices. To better clarify this point, let us recall some basic considerations on semiclassical- versus quantum-transport theory.

Whereas classical transport physics is based on the concept of a probability distribution which is defined over the phase space of the system, the concept of a phase-space distribution function in the quantum formulation of transport is difficult, since the non-commutation of the position and momentum operators (the Heisenberg uncertainty principle) precludes the precise specification of a point in phase space. However, within the formulation of quantum mechanics, various formalisms based on density matrices, Wigner functions, Feynman path integrals and Green's functions have been developed [4]. These embrace the quantum nature of transport; moreover, in recent years, each technique has been utilized to address key aspects of quantum transport in semiconductors. At present, there is no unifying, user-friendly approach to quantum transport in semiconductors. Density matrices, and the associated Wigner function approach, Green's functions, and Feynman path integrals all have their application and computational strength and weakness, and all their are equivalent representations of the quantum nature of transport. In the present work the density-matrix and Wigner-function formalisms will be employed. This choice is due to the fact that the "open system problem" that here is faced, is better managed using such an approach; Indeed the density-matrix formalism is extremely useful to show the degree of quantum coherence of the system under investigations while the Wigner-function picture is the ideal instrument to describe real-space quantum devices. Such a choice will be better understood looking in more detail to the problem of open systems, i.e., systems with open spatial boundaries.

Open systems

The most interesting products of micro- and nanoelectronics technology are systems that operate far from equilibrium. A closer inspection of a few examples of such systems reveals that they are generally open, in the sense that they exchange matter with their environment. The present work is aimed at developing a fully microscopic theory to describe open quantum systems starting from the so-called Semiconductor Bloch equations, namely the equations that describe the coherent versus incoherent dynamics of a closed quantum system. In the context of the present work, an open system is a system that exchange locally particles with its environment. Moreover, we wish to focus upon its far-from-equilibrium behaviuor, and thus the specific definition of open system will be further restricted to describe a system coupled to at least two separate particle reservoirs, so that a non-equilibrium state may be created and maintained. To specify such a system we must regard it as occupying a finite region of space, and thus the exchange of particles must consist of a current flowing through the system surface which is taken to be the boundary of the system. Anyway, it is important to point out that the distinction between closed and open systems depends upon how one chooses to partition the universe into the system of interest and everything else (such partitioning is implicit in the analysis of every physical problem). The physics of closed systems is certainly simpler than that of open systems, because closed systems obey global conservation laws, while open systems, in general, do not. In the well established techniques of physical theory one often encounters artifices, usually in the form of periodic boundary conditions, which assure the "closure of the circuit". The central point of the present discussion is that it is frequently necessary to subdivide a complex system (which might be reasonably regarded as closed) into smaller components which, viewed individually, must be regarded as open ones. Thus, the more applied disciplines of the physical sciences must often deal at some level with the concept of an open system. There are many techniques [5] for dealing with open systems in field such as fluid dynamics, neutron transport, and electronics. All these fields are concerned with the transport of (usually) conserved particles. The transport phenomena are described by transport equations at a kinetic, hydrodynamic or microscopic level which are either differential or integro-differential equations. Such equations require boundary conditions, and it is in these boundary conditions that the openness of a system is described. For the case of electronic and optoelectronic devices the connection to the external circuit is accomplished by some sort of contact. In solid state electronics the most frequently used type of contact is the ohmic contact, an interface between a metallic conductor and a semiconductor which permits electrons to pass freely.

Our aim is to analyse in detail the problem of openness in the present sense with also the possibility to consider energy-relaxation and dephasing processes within the device active region. More specifically, our analysis will allow us to point out and overcome some basic limitations of the conventional Wigner-function formalism (Model 1); this will be accomplished by introducing a Generalized Weyl-Wigner approach, able to remove such anomalies, thus recovering typical results of partially phenomenological models. In this context we shall propose a theoretical scheme where the boundary conditions are described via a source term, i.e., a term representing the particles entering the simulated region from its spatial boundaries. In particular, we shall propose two fully equivalent theoretical models able to describe adequately an open quantum device: the first one (Model 2) is characterized by a non-diagonal source term (i.e., coherent source) while the second one (Model 3) is characterized by a diagonal source term. From our analysis we shall conclude that Model 3 is the most appropriate one to describe transport phenomena in open quantum systems, since from a physical point of view this amounts to assume a thermal, i.e., diagonal, carrier injection from the device spatial boundaries. Anyway, our results will show a total agreement between Model 2 and Model 3.

Chapter 2

Semiclassical Transport Theory

2.1 Fundamentals

A condensed-matter system like a crystalline solid is typically characterized by a huge number of degrees of freedom, of the order of 10^{22} electronic and cristalline coordinates per cubic centimeter. The *microscopic configuration* or *microscopic state of the electronic system* is described in classical terms by specifying momentum and position of each particle at a given time; This means that for N electrons, we need to specify $3N + 3N$ coordinates, which corresponds to a point in the so called phase space Γ, namely a $6N$ degrees-of-freedom phase-space. In other words, a point in the Γ-space describes the microscopic state of all the N electrons in the system.

It is important to notice how different microscopic states (corresponding to different points in Γ-space) may correspond to the same macroscopic state of the system. For example, the condition that an electronic gas fills a given volume does not prevent to dispose the particles in this volume in infinitely different ways, i.e., by means of macroscopic measures, it is not possible to distinguish between two different microscopic states satisfying the same macroscopic conditions. Therefore, dealing with a gas subject to particular macroscopic constrains, this in general does not identify a specific microscopic state, but rather an infinite number of macroscopically equivalent microscopic states. Such a collection of states is usually referred to as *statistical ensemble*. It is important to point out that the members of an ensemble can be regarded as virtual copies of a system that do not interact one another.

The mathematical instrument which describes the concept of statistical ensemble in classical mechanics is the *distribution function* $\rho(q,p,t)$ with $q \equiv q_1, q_2, q_3, ..., q_{3N}$ and $p \equiv p_1, p_2, p_3, ..., p_{3N}$ so that:

$$dN = \rho(q,p,t)\ d^{3N}q d^{3N}p \tag{2.1}$$

represents the infinitesimal number of Γ-points within the infinitesimal volume $dV = dq^{3N}dp^{3N}$. It follows that a statistical ensemble is completely described by $\rho(q,p,t)$.

Given the distribution function ρ its time-evolution is dictated by the Hamilton equations:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{2.2}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{2.3}$$

with $i = 1, 2, ..., 3N$ and where $H = H(q_1, q_2, ..., q_N, p_1, p_2, ..., p_N)$ is the classical Hamiltonian of the system. Such equations describe the time evolution of a Γ-point, clearly showing its intrinsic invariance under time reversal.

Generally speaking, by looking at the dynamics of the distribution function $\rho(q,p,t)$, it is possible to verify that[1]:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3N} \Big(\frac{\partial \rho}{\partial q_i}\dot{q}_i + \frac{\partial \rho}{\partial p_i}\dot{p}_i \Big) = \frac{\partial \rho}{\partial t} + \{\rho, H\} = 0 \tag{2.4}$$

This equation is called *Liouville equation* [6]. It can be also written as:

$$\frac{d\rho(p,q,t)}{dt} = 0 \tag{2.5}$$

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[1] Here was used the Poisson bracket formalism.

This means that the density of Γ-points along the classical trajectory is constant in time, i.e., its total or hydrodynamic time derivative is equal to zero.
The Liouville equation can be considered as a "generalized equation" in the sense that it describes a statistical ensemble of identical systems in all possible microscopic configurations.

Starting from the notion of statistical ensemble in Γ-space, it is useful to introduce the concept of *single-particle distribution function* $f(\mathbf{r}, \mathbf{k}, t)$ so that:

$$dN = f(\mathbf{r}, \mathbf{k}, t)\ d^3\mathbf{r} d^3\mathbf{k} \tag{2.6}$$

is the number of particles inside the volume $d^3\mathbf{r} d^3\mathbf{k}$. The new single-particle phase space $\mathbf{r}, \mathbf{k}$ is called *space* μ (it is a six coordinate space). A μ-point represents the state of a single particle.

It is important to stress the differences between the Γ and the μ-space: the former describes the fully microscopic state of a N-particles system, the latter describes single-particle properties only within the so-called kinetic picture. The general procedure that allows to move from the Γ to the μ-space is called *reduction procedure.*

As a starting point, let us discuss the form of $f(\mathbf{r}, \mathbf{k}, t)$ at equilibrium. To address this problem, it is necessary to write down the equation of motion for $f(\mathbf{r}, \mathbf{k}, t)$. In order to get a closed equation for the single-particle distribution function, a number of approximations (discussed below) are needed. The resulting dynamical equation is called Boltzmann equation; the latter can indeed describe adequately the time evolution of $f(\mathbf{r}, \mathbf{k}, t)$ within our single-particle phase-space. In this respect, the Boltzmann equation can be regarded as the Liouville equation reduced to the μ-space.

Before entering into deep aspects of the Boltzmann equation, it could be useful to face the apparent contradiction between the intrinsic time reversibility of the Hamilton equations and the typical irreversibility of the Boltzmann-equation picture. This can be easily understood considering the fact that within the single-particle picture we describe the interaction of the generic particle with other degrees of freedom in average (i.e., statistical) terms. This is the origin of the irreversibility previously mentioned. This feature is formally expressed by the so called $\mathcal{H}$-*theorem* [7]. In fact, starting from the single-particle distribution function $f(\mathbf{r},\mathbf{p},t)$ we can define the quantity:

$$\mathcal{H}(t) \equiv -\int d\mathbf{r}d\mathbf{p}f(\mathbf{r},\mathbf{p},t)\ln f(\mathbf{r},\mathbf{p},t) \tag{2.7}$$

which is a measure of the system

$$\frac{d\mathcal{H}}{dt} \geq 0 \tag{2.8}$$

Only when $f(\mathbf{r},\mathbf{p},t)$ is the equilibrium distribution function we have $d\mathcal{H}/dt = 0$. It is then evident the apparent discrepancy between microscopic description (Hamilton equations) and kinetic picture ($\mathcal{H}$ theorem). The solution of such issue is that $d\mathcal{H}/dt$ is not necessarily a *continuous* function in time, so on a short (i.e., microscopic) time-scale it can also decrease. Then, by invoking the Poincaré theorem ("A finite energy system in a finite volume, will come back to the initial state after a long-enough time interval"), one can assert that the apparent discrepancy is thus removed.

2.2 Boltzmann equation

Semiclassical transport theory is applied to a wide variety of problems within the frame of nonequilibrium charge transport in semiconductors. The analysis of the electron motion in such systems should account for two different aspects:

1) deterministic or free (from scattering) evolution;

2) stochastic or scattering dynamics.

In the first case, the carrier dynamics is described in semiclassical terms: it is possible to predict the position $\mathbf{r}$ and the momentum $\mathbf{k}$ of a particle subject to external electric and/or magnetic fields. For the case of charge transport in semiconductors, this requires the knowledge of the electronic band structure, namely the dispersion relation $E_n(\mathbf{k})$, n being the band index. The resulting semiclassical equations of motion are as follows:

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{d}{d\mathbf{k}}E_n(\mathbf{k}) \tag{2.9}$$

$$\frac{d\mathbf{k}}{dt} = \frac{1}{\hbar}\mathbf{F}(\mathbf{r},\mathbf{k}) = \frac{q}{\hbar}[\mathbf{E}(\mathbf{r},t) + \frac{1}{c}\mathbf{v}_n(\mathbf{k})\,\mathbf{x}\,\mathbf{H}(\mathbf{r},t)] \tag{2.10}$$

where the equations represent respectively the carriers group velocity and the applied external force on the carrier.

Let us come to the stochastic or scattering dynamics. The scattering model commonly employed is the result of a number of different assumptions/approximations. Contrary to the deterministic evolution previously considered, the description of scattering dynnamics starts from quantum mechanics.

More specifically, in order to elucidate the limitations of the Boltzmann transport theory and to describe adequately the fundamental physical processes necessary to understand transport in solids, especially with regard to submicron and ultrasubmicron electronics, the basic assumptions and issues relevant to the Boltzmann transport equation (BTE) are reviewed.

As anticipated, the transport properties of carriers in bulk crystalline solids are derived from a probability distribution function $f(\mathbf{r},\mathbf{k},t)$. This function is defined as proportional to the density of particles in the reduced or single-particle phase space. For a homogeneous solid in thermodynamic equilibrium, $f(\mathbf{r},\mathbf{k},t)$ is $f_0[E(\mathbf{k})]$, where f_0 is the Fermi-Dirac distribution function at temperature T. For nonequilibrium conditions, the distribution function can be found by solving the Boltzmann transport equation:

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}\cdot\frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{2.11}$$

where the rhs term represents the change of the distribution function due to scattering events. As pointed out before, such term is described via time-dependent second-order perturbation theory of quantum mechanics within the well-known Fermi's golden-rule approximation. As a result one obtains:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{k'} \left\{ f(\mathbf{r}, \mathbf{k}', t) W(\mathbf{k}', \mathbf{k}; \mathbf{r}) - f(\mathbf{r}, \mathbf{k}, t) W(\mathbf{k}, \mathbf{k}'; \mathbf{r}) \right\} \tag{2.12}$$

where $W(\mathbf{k}, \mathbf{k}'; \mathbf{r})$ is the transition rate from state $\mathbf{k}$ to $\mathbf{k}'$ and depends on the details of the scattering mechanisms [8], e.g., electron-phonon scattering, electron-impurity scattering, etc.

Using the microscopic reversibility of the scattering process, it can be show that for $f = f_0(E)$ we have $(\partial f/\partial t)_{coll} = 0$, thus ensuring that, for a homogeneous solid in thermodynamic equilibrium (i.e., where all terms on the left-hand side of BTE are zero), the solution of the Boltzmann transport equation reduces to the usual equilibrium distribution function. If we are dealing with low density electrons/holes ($f(\mathbf{r}, \mathbf{k}, t) << 1$), then the terms in brackets in the collision term can be replaced by unity, thus significantly simplifying the scattering term.

In presenting an elementary derivation of the Boltzmann equation, we consider a group of carriers in the volume element $d\mathbf{r}d\mathbf{k}$ in phase space (the number of such electrons for a given spin direction is $f(\mathbf{r}, \mathbf{k}, t) d\mathbf{r} d\mathbf{k}/(2\pi h)^3$). At a time δt later, with no scattering, these carriers move to positions $\mathbf{r} + \delta\mathbf{r}$, $\mathbf{k} + \delta\mathbf{k}$ in a volume $d\mathbf{r}'d\mathbf{k}'$. For a short enough time δt, the volume element in phase space will not change ($d\mathbf{r}d\mathbf{k} = d\mathbf{r}'d\mathbf{k}'$) since all the electrons in the original volume element have essentially the same position and quasimomentum, and therefore the changes in $\delta\mathbf{r}$ and $\delta\mathbf{k}$ for all electrons are the same to the lowest order. However, if collisions are allowed at the rate of $(\partial f/\partial t)_{coll}$, then the distribution function evolves as:

$$f(\mathbf{r} + \delta\mathbf{r}, \mathbf{k} + \delta\mathbf{k}, t + \delta t) = f(\mathbf{r}, \mathbf{k}, t) + \delta t \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{2.13}$$

Expanding such a equation, one obtains:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \mathbf{F} \cdot \nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{2.14}$$

According to the relation that links $\mathbf{p}$ to $\mathbf{k}$, that is $\mathbf{p} = \hbar\mathbf{k}$, it is easy to see that the equation just written is exactly the equation (2.11).

The right-hand side of (2.14) can be easily obtained by noting that $(\partial f/\partial t)_{coll}$ should be merely the rate at which electrons from all other states $\mathbf{k}'$ are scattered into state $\mathbf{k}$, minus the rate at which electrons in state $\mathbf{k}$ are scattered into other state $\mathbf{k}'$, all of which are evaluated at $\mathbf{r}$ and t. If $W(\mathbf{k}', \mathbf{k})$ is the transition rate from a filled state $\mathbf{k}'$ to an empty state $\mathbf{k}$, then one expects the transition rate from a state with fractional occupancy $f(\mathbf{r}, \mathbf{k}', t)$ to a state of fractional occupancy $f(\mathbf{r}, \mathbf{k}, t)$ to be given by the first term in 2.13, with the factor $1 - f(\mathbf{r}, \mathbf{k}, t)$ giving the fraction of states which are empty. This satisfies the exclusion principle that transitions to filled states are forbidden. Similarly, the second term gives the scattering from states $\mathbf{k}$ to $\mathbf{k}'$.

Despite the apparent simplicity of the above derivation, it has significant deficiencies. First, because of the uncertainty principle, the function $f(\mathbf{r}, \mathbf{k}, t)$ does not have a precise meaning as a probability function in both $\mathbf{r}$ and $\mathbf{k}$. In fact, if wave packets are formed, the $\Delta x \Delta k \sim 1$, and if the unacertainty in Δk is to be only a small fraction of $\mathbf{k}$ (so to be able to describe a state with well-defined $\mathbf{k}$), then the spread of the wave packet in space Δx must be many electron wavelengths long. This is a particularly serious restriction in semiconductors, where the thermal de Broglie wavelength can be quite large. Thus, the BTE cannot be expected to give a correct description of the spatial variation of the distribution if it changes significantly over several wavelenghts of a typical carrier, as can be expected to occur if the force $\mathbf{F}$ has such a spatial variation.

Second, the picture employed treats the electrons as essentially free particles only, which are occasionally scattered by phonons, impurities, imperfections, and are not affected between collisions. However, the electrons interacting with additional potentials will alter their $E(\mathbf{k})$ function and, hence, their velocity.

Third, the use of an external field $\mathbf{F} = \hbar \, d\mathbf{k}/dt$ that is implicit in 2.14, is justified only if $\mathbf{F}$ is essentially constant (i.e., its spatial variation is very slow with respect to the packet wavelenght) over the width of the electron wave packet, which can be large for semiconductor, as indicated above. The violation of the effective-mass assumption also implies that interband

and nonparapolicity effects must be considered if the field is turned on too rapidly, and this can be important for superlattices having very small band gaps.

Fourth, the assumption that the scattering takes place locally in space and time is incorrect since the scattering potentials are extended in space and take a finite amount of time to complete. During a scattering process, an electron will have its energy changed because it is being accelerated by the force $\mathbf{F}$. Thus the assumption that the effects of the field and the effects of collisions can be treated independently is not entirely accurate; such an assumption can be expected to break down when the energy change due to the field acting over the collision time τ_c is of the order of E, the average energy of an electron.

Fifth, the transition rate is generally calculated by assuming that it originates from an incoherent sum of single scattering events. However, if the scatters are dense (i.e., more than one within a de Broglie wavelength), multiple scattering effects are possible.

Sixth, the electron-electron interaction can become significant for dense systems, such as quantum confining wells.

In conclusion, the validity of the semiclassical approach, and of the BTE, is ascribed to the fulfillment of the following conditions:

a) the wave packet related to a carrier can be considered of small dimensions in both real and momentum space, such that a particle can be related to a defined point in phase space $(\mathbf{r}, \mathbf{k})$; That means that during the free flight between two successive collisions, carriers are considered as classical particles. In order that this approximation can be acceptable, the wave packets momentum uncertainty $\Delta\mathbf{k}$ must be less than their average momentum $\mathbf{k}$ and, at the same time, a position uncertainty $\Delta\mathbf{r}$ much less than the free path l:

$$\Delta k << k, \Delta r << l \tag{2.15}$$

From the Heisenberg uncertainty principle:

$$1 \sim \Delta k \Delta r << k * l \sim \frac{1}{\hbar}\frac{p^2}{m}t \sim \frac{1}{\hbar}KTt \qquad (2.16)$$

where t is the time between two successive collisions, K is the Boltzmann constant and T the temperature. From the above relations we obtain:

$$t >> \frac{\hbar}{KT} \sim 10^{-13} sec \qquad (2.17)$$

at ordinary temperatures.

b) Collisions are assumed instantaneous in time and pointlike in space; this assumption allows to give a simple form to the collision integral entering the BTE. Since the interactions between the particles and the scattering agents have finite durations, this assumption is not correct in general, not even in classical theory. In the case of weak coupling, when scattering events are sufficiently rare, the duration of a collision may be negligible with respect to the free-flight time between two successive collisions, and the assumption may be reasonable. In order to estimate the requirement for such a condition to be fulfilled, the collision duration has to be estimated. This estimate is somewhat arbitrary, because the concept of collision duration is ill defined. Anyway it is possible to obtain an expression to evaluate the collision duration and such results is:

$$t_{coll} \sim \frac{\hbar}{KT} \qquad (2.18)$$

Therefore, the requirement that the collision duration is much shorter than the time between collisions coincides with the above requirement done in (a).

From the points discussed above, it is clear that the critical parameter for evaluating the applicability of the semiclassical transport theory is the time t between collisions in the semiclassical theory itself.

Hence, such considerations suggest that it is extremely desirable to derive a transport equation from more general quantum mechanical considerations, as shown in the next chapter.

2.3 From closed to open systems: semiclassical point of view

Speaking about a *closed system*, this means to identify the system of interest as the whole system, namely it cannot exchange matter or energy with the environment, since the environment is not definite or, better, it is inside the system. That implies that the study of close systems is simpler than that of open systems, indeed the formers obey global conservation laws, while the latters, in general, do not.

In the analysis of theoretical systems one often has recourse to artifices, as periodic boundary conditions, which assure the closure of the systems at least from the point of view of the theoretical modelling, if not of the system itself. For example it is useful to reduce the continuous infinite **k** space into a discrete infinite space, to be able to manage it from a computational point of view, by introducing the Born-Von Karman conditions, that is periodic boundary conditions.

Nevertheless that kind of conditions do not assure the closure of the system itself, in fact to do that it is necessary to understand where to localize the borders of the system of interest to understand where begins the environment. That kind of action could seem simple but it is important to emphasize the crucial role kept by it inasmuch as the way to partition the whole system determines on which effective system one will deal with.

Since the existing theoretical work on open systems consists primarily of the definition of boundary conditions on transport equations, it is appropriate to examine various approaches to transport theory to see how they have dealt with this issue. This examination will center upon electron-transport theory, because we wish to include quantum-coherence effects in the theory, and these are much more prominent in systems of electrons than in systems of more massive particles.

Chapter 3

Quantum Transport Theory

3.1 Fundamentals

In the previous chapter we have already pointed out the need of introducing a fullly quantum-mechanical transport theory for the description of charge dynamics on very short space- and time-scales, for which the semiclassical description previously introduced comes out to be unadequate. Indeed, the classical *single-particle distribution function*, as such, can not adequately describe quantum-correlation phenomena in the space- and/or time-domain, due to the neglect of the Heisenberg uncertainty principle. Aim of the present chapter is to discuss how to extend the semiclassical scenario previously analized to properly describe interference phenomena in semiconductor-based quantum devices.

3.1.1 Landauer-Büttiker approach

A fundamental approach able to qualitatively describe the open character of transport in quantum devices is the one proposed by Landauer and Büttiker [11] [12] [13]. Within this approach, energy-relaxation/dephasing processes do not occur inside the device, but dissipation is accounted for via coupling to two or more ideal charge reservoirs. The conductance of such a structure is then expressed in terms of the quantum-mechanical transmission coefficients of the confinement potential profile. The ideal reservoirs have properties analogous to those of a blackbody: they absorb without reflection any electron leaving the system and inject into the device active region an equilibrium thermal distribution. We shall see that such a picture is indeed the qualitative starting point for constructing more refined open-system models. However, we stress that this approach does not specify the boundary conditions within a physical boundary-value problem. The boundary conditions are actually applied to the Schödinger equation —i.e., to the carrier wavefunction— and correspond to the asymptotic conditions upon which the formal theory of scattering is based. The traditional approach is to expand the unknown electron wave function in a set of travelling waves, which correspond to the physical electron states in the asymptotic regions. This implicitly sets the boundary conditions employed in such an analysis. Alternatively, for the study of electron transport within a finite region of space, purely numerical techniques for solving Schrödinger's equation in a closed-system perspective are usually employed. The resulting set of electron states is then used as a basis on which the physical phenomenon of interest is described; to this end it is imperative to impose on such basis set proper boundary conditions compatible with the open-system character of our quantum device.

Let us consider the steady-state regime for a one-dimensional system extending over the interval $0 \leq x \leq l$ inside which there is a generic potential profile (that represents the quantum device). In general, one seeks wave functions corresponding to travelling waves incident from either left or right. These states will include a reflected component which appears at the same boundary as incident wave, and a transmitted component which appears at the opposite boundary. For example, for an eigenstate incident from left, we have:

$$\psi(x) = Ae^{ik_0x} + Be^{-ik_0x} \qquad \text{for x} \leq 0 \tag{3.1}$$

$$\psi(x) = Ye^{ik_lx} + Ze^{-ik_lx} \qquad \text{for x} \geq l \tag{3.2}$$

where $Z = 0$ (for the hypothesis to have a left-incident wave function). The potential profile inside the region $[0, l]$ is approximated by a step-like potential; this approximation is as better as we consider a high number N of step-potentials. For this reason, the region $0 \leq x \leq l$ can be described by:

$$\psi(x) = C_1 e^{ik_1 x} + D_1 e^{-ik_1 x} \qquad \text{for x} \in \text{I-step-potential} \tag{3.3}$$

$$\psi(x) = C_2 e^{ik_2 x} + D_2 e^{-ik_2 x} \qquad \text{for x} \in \text{II-step-potential} \tag{3.4}$$

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$$\psi(x) = C_N e^{ik_N x} + D_N e^{-ik_N x} \qquad \text{for x} \in \text{N-step-potential} \tag{3.5}$$

In this treatment we have $2N+3$ unknown quantities, but thanks to the continuity conditions on the $\psi(x)$ function and on its first derivative $d\psi(x)/dt$ ($2N+2$ conditions), it is possible to write down them in terms of A, that finally can be obtained thanks to normalization condition. Obviously this approach is problematic since it requires to deal simultaneously with a large number of unknown quantities. To overcome this limitation, the problem can be rewritten in terms of the *scattering matrix* S, that is a mathematical instrument that allows to write down out-going states in terms of in-coming states. By using the usual terminology in a compact form one obtains:

$$\begin{pmatrix} B \\ Y \end{pmatrix} = S \begin{pmatrix} A \\ Z \end{pmatrix} \tag{3.6}$$

Still, this treatment is unfortunately not adequate to describe our system, indeed the hypothesis to inject within the device either from left or from right precludes the possibility to have simultaneously both A and Z term. Therefore, it is better to consider the so called *transfer matrix* T that relates the right-quantum-device unknown quantities to the left-quantum-device quantities. Hence one obtains:

$$\begin{pmatrix} Y \\ Z \end{pmatrix} = T_{tot} \begin{pmatrix} A \\ B \end{pmatrix} \tag{3.7}$$

where T_{tot} is the *total* transfer matrix. In fact it is important to notice that the transfer-matrix approach must be used to connect adjacent zones with different potentials, going from right to left of the whole potential profile (being under the hypothesis to inject from left), and the product of all the specific transfer matrix gives T_{tot}. In a compact form we get:

$$\begin{pmatrix} C_N \\ D_N \end{pmatrix} = T_l \begin{pmatrix} Y \\ Z \end{pmatrix} \tag{3.8}$$

$$\begin{pmatrix} C_{N-1} \\ D_{N-1} \end{pmatrix} = T_{N,N-1} \begin{pmatrix} C_N \\ D_N \end{pmatrix} \tag{3.9}$$

$$\begin{pmatrix} C_{N-2} \\ D_{N-2} \end{pmatrix} = T_{N-1,N-2} \begin{pmatrix} C_{N-1} \\ D_{N-1} \end{pmatrix} \tag{3.10}$$

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$$\begin{pmatrix} C_1 \\ D_1 \end{pmatrix} = T_{2,1} \begin{pmatrix} C_2 \\ D_2 \end{pmatrix} \tag{3.11}$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = T_0 \begin{pmatrix} C_1 \\ D_1 \end{pmatrix} \tag{3.12}$$

with $T_{tot} = T_l T_{N,N-1} T_{N-1,N-2} ... T_{2,1} T_0$.
Note that the matrix T depends on the wavevector k and carrier effective mass m only.

The Landauer approach previously recalled has successfully described a number of quantum phenomena [14] [15]. However, it is important to recognize that these phenomena occur only under a very restricted range of circumstances [16]. The reason for this is not only the fragility of quantum interference effects as such, but rather the fact that the elementary Schrödinger picture is not properly adequate to describe quantum-interference effects in the presence of energy-relaxation and dephasing phenomena. That is as much true as the temperature rises (indeed a lot of states may participate in the conduction), in particular in situations far from equilibrium. A satisfactory treatment of far-from-equilibrium phenomena requires hence an approach at a level of sophistication at least equal to that of the *semiclassical kinetic theory*.

3.1.2 Quantum kinetic approach

In the first chapter we have introduced the space Γ, namely the $6N$ phase-space, whose points represent in classical terms the *whole* system under investigation. However, such a detailed system description is usually not adequate, since we are often interested only in a *subspace* of the whole system. Thus, a generally accepted approach to the problems of statistical physics is to begin with the general theory of many-body (Γ space) dynamics and to proceed by deductive reasoning to a formulation that provides an answer for the problem of interest [17]. The steps of this deductive chain necessarily involve the introduction of extra assumptions in the form of suitable approximations. One may loosely categorize the level of approximation in terms of the independent variables required to specify the state of the system. The most detailed level is the fundamental many-body theory, which in principle requires a complete set of dynamical variables for each particle. This can be reduced to the kinetic level by restricting our attention to one-body properties (μ space). It may be necessary also to remove, i.e., to adiabatically eliminate, other dynamical variables of the system, such as photon or phonon coordinates, when the electron gas is the only subsystem of interest. The kinetic theory is expressed in terms of distribution function defined on a single-particle phase space, requiring one position and one momentum variable for each spatial dimension (in the quantum case, this corresponds to a couple of quantum numbers labelling the density operator). Finally, the hydrodynamic level of approximation is obtained by making some assumption about the form of the distribution function in momentum space, and integrating key quantities like carrier velocity and kinetic energy over k-space. Thus the hydrodynamic theory is expressed in terms of macroscopic quantities that are functions of position only.

Within the kinetic description previously recalled, the effects of degrees of freedom that are of less interest for a given problem are included implicitly in object such as collision operators or effective interaction potentials. For the case of electronic devices such auxiliary degrees of freedom should include electron coordinates outside the device, but within the external circuit. They also include all the excitations of the device material apart from the single-electron states (e.g., phonons, plasmons, etc.). Thus, the state of the system is usually described by a one-body density operator.

In the previous chapter the density function was introduced, in particular as the function that obeys the Boltzmann equation. As previously discussed, such an equation is appropriate to describe phenomena in a "semiclassical" world, that is in conditions where quantum effect are not very prominent. Now, because of the quantum nature of microscopic systems, it is nevertheless necessary to introduce a new mathematical instrument able to describe adequately quantum phenomena, namely phase coherence vs. energy-relaxation/dephasing processes. This instrument is called *single-particle density matrix* (see appendix A). In general, this can be written as

$$\rho(x, x', t) = \sum_k p_k \langle x|\psi_k(t)\rangle\langle\psi_k(t)|x'\rangle \tag{3.13}$$

where k labels a set of states and p_k are real-valued probabilities for the system in state $\psi_k(t)$. Since we will consider open systems in which the number of particles is not fixed, the usual convention for the normalization of $\rho(t)$ ($Tr\rho(t) = 1$) is not useful. Instead we shall adopt a normalization convention such that $\rho(x, x', t)$ gives the actual particle density. More formally, $\rho(x, x', t)$ is a one-body reduced density operator which is defined on a single-particle Hilbert space. The complete density matrix defined on the many-particle Fock space may still be normalized to unity.

For a system described by a simple single-particle Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{3.14}$$

the time evolution of the single-particle density matrix is again described by the well-known Liouville-von Neumann equation:

$$i\hbar\frac{\partial\rho}{\partial t} = [H, \rho] = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2}\right]\rho + [V(x) - V(x')]\rho \equiv \mathcal{L}\rho \tag{3.15}$$

where $\mathcal{L}$ is the Liouville superoperator[1]. The simplest approach to describe the behaviour of

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[1] Anything that generates linear transformation on a density operator.

open systems is to apply the Liouville equation to a *finite* spatial domain representing the system of interest an to apply boundary conditions that model the open nature of the system. The difficulties and ultimate success of this approach depend on the effect that such boundary conditions have upon the properties (particularly the eigenvalue spectrum) of the Liouville superoperator.

Quantum kinetic theory appears to be the simplest level at which one may consistently describe both quantum interference and irreversible phenomena [19]. The only available simple levels, i.e. requiring few independent variables, are hydrodynamic models and scattering-theory quantum mechanics.

However, hydrodynamic approaches provide no means to describe quantum effects such as resonance phenomena since they retain no information on the distribution of particles with respect to energy or momentum. On the other hand. if one attempts to include irreversible processes within the framework of elementary quantum mechanics (scattering-theory), the probabilistic continuity equation is most often violated. Irreversible processes will generally result in the time dependence of some physical observable showing an exponential decay. The only time dependence provided by elementary quantum mechanics is $e^{-iEt/\hbar}$ dependence of the wave function. Nevertheless an exponential decay (that, as stressed, is related to irreversible processes) implies that the electron exponentially disappears, violating charge conservation. Moreover, violations of charge continuity still occur when the irreversible processes are described by the Fermi golden rule inside the frame of the lowest order theory perturbations. In this scheme, indeed, the density matrix is valid only in its diagonal or semiclassical limit, i.e., neglecting any coherence effect. To better clarify this point, let us consider a possible density matrix definition in x-space

$$\rho(x, x', t) = \sum_i p_i(t)\psi_i(x)\psi_i^*(x') \tag{3.16}$$

where we assume that the density matrix is diagonal in the basis of the eigenstates ψ_i of the Hamiltonian and that the time-evolution is Boltzmann-like. The equation that dictates the dynamics for $p_i(t)$ is

$$\frac{dp_i}{dt} = \sum_j [p_j W_{ji} - p_i W_{ij}] \tag{3.17}$$

where the W_{ji} are the golden-rule transition rates. Let us consider the transition from a state i to a state j which have different spatial distribution: $|\psi_i(x)|^2 \neq |\psi_j(x)|^2$. Because of the "only diagonal density matrix description" given by scattering-theory, let us consider the rate of change of the diagonal density

$$\frac{\partial}{\partial t}\rho(x,x,t) = \frac{\partial p_i}{\partial t}|\psi_i(x)|^2 + \frac{\partial p_j}{\partial t}|\psi_j(x)|^2 = [p_i(t)W_{ij} - p_j(t)W_{ji}][|\psi_i(x)|^2 - |\psi_j(x)|^2] \tag{3.18}$$

However, i (similarly for j) is an eigenstate of H, which means that $\langle i|J|i\rangle$ is constant. Now, the rate of change of the density is equal to zero if either of the two bracketed terms in Eq.(3.18) is zero. In thermal equilibrium the first term is zero in virtue of the detailed-balance principle, but away from equilibrium it is, in general, nonzero. The second term will be zero if the probability distributions of the eigenstates i and j are identical. This happens for very special cases only, most notably for the plane-wave states of a free particle.

Thus the assumption that the density matrix has the form (3.16) for a far-from-equilibrium systems will lead, in general, to a violation of the continuity equation. To maintain consistency with the continuity equation, it is imperative to properly include off-diagonal elements of the density matrix (in the eigenbasis of the Hamiltonian) [19]. Anyway, the expression that we shall use to represent the density matrix, will be not the Eq.(3.16) but

$$\rho(x,x',t) = \sum_i p_i \psi_i(x,t)\psi_i^\dagger(x',t)$$

Here the time-evolution is inside the wave function ψ and, as shown in Appendix A, it can be demonstrate that

$$\frac{\partial \rho(x,x,t)}{\partial t} = 0$$

In conclusion, we remember that a theory that describes the evolution of the complete (diagonal plus non-diagonal) single-particle density matrix is by definition a quantum kinetic theory.

Open boundaries and time-irreversibility

The usual way to describe the effects of dissipative or irreversible processes at the kinetic level is to add a collision term to the Liouville equation (3.15) to obtain the Boltzmann equation. This is a valid procedure as long as the dissipative processes are sufficiently weak that the motion of the particles can be viewed as periods of free flight interrupted by collision events. Such a term takes its simplest form for interactions between the particles of interest (i.e., electrons) and quasiparticles that either are spatially fixed (such as impurities in solids) or can be modelled as components of a thermal reservoir (such as phonons). In this case, within the Markov approximation and low-density limit the collision term reduces to a simple linear superoperator, and we can recover the Boltzmann equation as diagonal part of

$$\frac{\partial \rho}{\partial t} = \mathcal{L}\rho + \mathcal{C}\rho \tag{3.19}$$

where $\mathcal{C}$ is the collision superoperator (it is the Boltzmann collision term).

A feature of irreversible systems is the existence of stable stationary states, which can be either the equilibrium state or a nonequilibrium steady state if the system is driven by external forces. To describe the reaching of such a steady state the superoperator $\mathcal{L} + \mathcal{C}$ must have eigenvalues with negative real parts. In the usually studied case the Liouville superoperator is anti-Hermitian, which corresponds to purely imaginary eigenvalues. On the contrary the collision operator $\mathcal{C}$ introduces the negative real parts of the eigenvalues. Physically, we expect that there should be no eigenvalues with positive real parts, because these would correspond to exponentially growing modes, and the system would be intrinsically non stable. The presence of eigenvalues with negative real parts together with the absence of eigenvalues with positive real parts implies that the system is time irreversible. This requests play a very important role since it determines the sort of boundary conditions that can be used to model open systems.

In fact it can be shown that *the time irreversibility enters through the open-system boundary conditions* [5].

Boundary conditions

To describe the behavior of an open system, we shall consider an approach in which the spatial domain is considered to be finite, corresponding to the extent of the system, and boundary conditions are applied which permit particles to pass into and out of the system. As previously stressed, the boundary conditions must be time irreversible in themselves to guarantee the correct analysis of open systems. A physically appealing way to achieve such irreversibility is to distinguish between particles moving into the system and those moving out of the system. It is then reasonable to expect that the distribution of particles flowing into the system depends only upon the properties of the reservoirs to which the system is connected, and that the distribution of particles flowing out of the system depends only upon the state of the system. The behaviour of the reservoirs is thus analogous to that of an optical blackbody. This picture leads to a fully acceptable model of open system.

To implement the picture just described, we should apply the boundary conditions

$$\begin{aligned} f(z_{left},k)|_{k>0} &= f^{left-boundary}(k) \\ f(z_{right},k)|_{k<0} &= f^{right-boundary}(k) \end{aligned} \tag{3.20}$$

where z_{left} and z_{right} represent the boundaries of the system under investigation, namely the open system, and $f^{boundary}$ is the distribution function of the reservoir to the left or to the right of the device. These boundary conditions are not invariant under time reversal.

3.1.3 Phenomenological approach

An important approach to open systems, that can be adequately included within the frame of microscopic transport (see next section), is represented by phenomenological boundary conditions. In such a scheme, the injection is completely delocalized inside the device, namely it is characterized by the absence of spatial coordinates inside the contacts. The reasons of such assumption are in the hypothesis that the injection involves electron wavepackets larger than the device itself, thus one can reasonably take a “plane-wave” limit. In other words, the smallness of the device leads to the assumption that electrons are injected as completely delocalized objects.

In order to generalize the Liouville equation to take into account the role played by the boundaries, we can add an open-boundary extra-term to the Liouville equation, similarly to the collision term considered in the previous section:

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}[\rho, H] + \left(\frac{\partial \rho}{\partial t}\right)\bigg|_{res} \tag{3.21}$$

The explicit form of the reservoir term is [20]

$$\left(\frac{\partial \rho_{\alpha\beta}}{\partial t}\right)\bigg|_{res} = -\gamma_\alpha[\rho_{\alpha\beta} - f^0_\alpha]\,\delta_{\alpha\beta} \tag{3.22}$$

being ρ_α the diagonal matrix elements of the reduced single-electron density matrix taken over electron states associated to the injection which it is related with; γ_α is the inverse of the device transit time for an electron in stateα; $f^0_\alpha = \left(e^{\frac{E_\alpha - \mu_\alpha}{k_B T}} + 1\right)^{-1}$ is the equilibrium carrier distribution in the external reservoirs.

The inclusion of diagonal contributions of the reservoir density matrix only is due to the fact that non-diagonal elements can be neglected in the hypothesis of carrier injection from a fully thermalized charge reservoir.

3.2 From close to open systems: microscopic approach

After a review of qualitative —i.e., partially phenomenological— approaches used to describe non-equilibrium carrier dynamics in open systems, let us now face the same problem from a fully microscopic point of view. In the following we shall demonstrate how it is possible to develop a theoretical scheme that is in a position to represent efficiently quantum effects in open-boundary systems.

The equation that governs the time evolution of the density matrix is the usual Liouville equation

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] \tag{3.23}$$

Obviously to solve such equation we need the explicit form of the Hamiltonian. The kinetic approach faced such point by considering the single-particle Hamiltonian form, how explicitly written in Eq.(3.15). The approach that we shall follow is different by the previous one, inasmuch as we are going to consider the *whole* system Hamiltonian.

3.2.1 Physical system

In order to study the transport properties of semiconductors, let us consider a gas of carriers in a crystal under the action of an applied electromagnetic field. Such physical system can be described by the following Hamiltonian:

$$H = H_c + H_p + H_{cc} + H_{cp} + H_{pp} \tag{3.24}$$

The first term describes the noninteracting-carrier system in the presence of the external electromagnetic field, while the second one refers to the free-phonon system. The last three terms describe many-body contributions: they refer, respectively, to carrier-carrier, carrier-phonon, and phonon-phonon interactions.

Since we are interested in the electro-optical properties as well as in the ultrafast dynamics of photoexcited carriers, the electromagnetic field acting on the crystal will be the sum of two different contributions: the high-frequency laser field responsible for the ultrafast optical excitation and the additional electromagnetic field acting on the photoexcited carriers on a longer time-scale. More specifically, we can denote these two contributions as

$$H_c = H_E + H_{cl} \tag{3.25}$$

where they describe, respectively, the carrier-static field and carrier-laser interaction.

Then, in first quantization, the Hamiltonian terms H_c can be written as

$$H_c = \frac{(-i\hbar\nabla_{\mathbf{r}} - \frac{q}{c}\mathbf{A}(\mathbf{r},t))^2}{2m_0} + q\varphi(\mathbf{r},t) + V^l(\mathbf{r}) \tag{3.26}$$

being $\mathbf{A}(\mathbf{r},t)$ the vector potential and $\varphi(\mathbf{r},t)$ the scalar potential corresponding to the external electromagnetic field, while V^l is the periodic potential due to the crystal.
To specify the two contributions H_E and H_{cl}, we can define the potentials as

$$\mathbf{A}(\mathbf{r},t) \equiv \mathbf{A}_1(\mathbf{r},t) + \mathbf{A}_2(\mathbf{r},t) \tag{3.27}$$

and

$$\varphi(\mathbf{r},t) \equiv \varphi_1(\mathbf{r},t) + \varphi_2(\mathbf{r},t) \tag{3.28}$$

where the terms labelled by “one” are associated to H_{cl} and the terms labelled by “two” are associated to H_E.

To simplify the carrier-laser interaction, we adopt the potential scalar gauge ($\mathbf{A}_1 = 0$), so that

$$H_{cl} = q\varphi_1(\mathbf{r},t) \tag{3.29}$$

where φ_1, under the dipole approximation, becomes

$$\varphi_1(\mathbf{r},t) = -\mathbf{E}_1(t)\cdot\mathbf{r} \tag{3.30}$$

being

$$E_1(t) = E_0(t)\cos(w_L t) \tag{3.31}$$

with $E_0(t)$ the amplitude of the light (i.e., gaussian) and w_L the frequency field.

In order to better represent the dynamics of the density matrix, let us write down the above expressions within the usual second quantization picture. By using the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$, one obtains:

$$H_c = \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r}) \left[\frac{(-i\hbar\nabla_\mathbf{r} - \frac{q}{c}\mathbf{A}(\mathbf{r},t))^2}{2m_0} + q\varphi(\mathbf{r},t) + V^l(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \tag{3.32}$$

and consequently H_E and H_{cl}.

Coming to the many-body contributions (H_{cc}, H_{cp}, H_{pp}), we should follow the same analysis seen for the single-particle contributions. Anyway, such a analysis is not necessary since our primary goal will be to study essentially the open system effects; therefore, we shall describe the many-body interactions in terms of the well-known $t_1 - t_2$ approximation[2].

3.2.2 Single particle approximation

In previous chapters we have discussed about the difference between statistical spaces Γ and μ. From our discussion it the impossibility to treat N particles systems (with N of the order of $10^{23} part/m^3$). For such a reason it is necessary to be able to reduce the problem to one that can be actually solved; Thus it was introduced the single particle space μ. For the same reason we must act on the Liouville equation (3.23). The approach that we shall follow is different from the one seen in section "kinetic approach", where the reduction procedure was done directly on the Hamiltonian, indeed now we shall reduce the density matrix ρ.

To this end, let us move to the second quantization picture. To do that we can write the field operators by using a basis $\{\phi_n(\mathbf{r})\}$:

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sum_n \phi_n(\mathbf{r})\hat{c}_n \\ \hat{\psi}^\dagger(\mathbf{r}) &= \sum_n \phi_n^*(\mathbf{r})\hat{c}_n^\dagger \end{aligned} \tag{3.33}$$

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[2] Within such an approximation scheme there exist a parameter t_1 describing the time necessary at the charge population to reach a steady state, and a parameter t_2 that simulates the decoherence time.

where $\hat{c}_n$ and $\hat{c}_n^\dagger$ represent, respectively, the destruction and creation of a carrier in state n.

To properly define/identify the single-particle density matrix ρ^{sp}, let us consider a single-particle operator $A(\mathbf{r})$ and let us write it in second quantization:

$$A^{sp} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) A(\mathbf{r}) \hat{\psi}(\mathbf{r}) = \int d\mathbf{r} \sum_\alpha \hat{c}_\alpha^\dagger \phi_\alpha^*(\mathbf{r}) A(\mathbf{r}) \sum_\beta \hat{c}_\beta \phi_\beta(\mathbf{r}) = \sum_{\alpha\beta} \hat{c}_\alpha^\dagger \hat{c}_\beta A_{\alpha\beta} \tag{3.34}$$

From Eq.(**??**), its mean value (both quantum and statistical) is

$$\overline{\langle A^{sp} \rangle} = Tr[\rho A^{sp}] = Tr\left[\rho \sum_{\alpha\beta} \hat{c}_\alpha^\dagger \hat{c}_\beta A_{\alpha\beta}\right] = \sum_{\alpha\beta} Tr\left[\rho \hat{c}_\alpha^\dagger \hat{c}_\beta\right] A_{\alpha\beta} \tag{3.35}$$

By defining the quantity

$$\rho_{\beta\alpha}^{sp} \equiv Tr[\rho \hat{c}_\alpha^\dagger \hat{c}_\beta] = \overline{\langle \hat{c}_\alpha^\dagger \hat{c}_\beta \rangle} \tag{3.36}$$

we get

$$\overline{\langle A^{sp} \rangle} = Tr[\rho^{sp} A^{sp}] \tag{3.37}$$

Thus it is important to point out the relation

$$\overline{\langle A^{sp} \rangle} = Tr[\rho A^{sp}] = Tr[\rho^{sp} A^{sp}] Tr[\rho^{sp} A^{sp}] \tag{3.38}$$

The meaning of such equation is very deep inasmuch as it has strong consequence in the calculation of observables mean value. Indeed it means that to find an expectation value of a single-particle quantity one does not need the *whole* density operator but it is enough to know the density operator of the system under investigation.

Space reduction

In more general terms, let us consider two different systems (1) and (2) and the global system (1) + (2), whose state space is the tensor product:

$$\mathcal{E} = \mathcal{E}(1) \otimes \mathcal{E}(2) \tag{3.39}$$

Let $\{|u_n(1)\rangle\}$ be a basis for $\mathcal{E}(1)$ and $\{|v_p(2)\rangle\}$ a basis for $\mathcal{E}(2)$; the kets $|u_n(1)\rangle|v_p(2)\rangle$ will constitute a basis for $\mathcal{E}$. The density operator ρ of the global system is an operator which acts over $\mathcal{E}$. We shall now show how to construct from ρ an operator $\rho(1)$ (or $\rho(2)$) acting only over $\mathcal{E}(1)$ (or $\mathcal{E}(2)$) which will enable us to make all the physical predictions about measurements bearing only on system (1) or system (2). This operation will be called a partial trace with respect to (2) (or (1)).

Let us introduce the operator $\rho(1)$ whose matrix elements are:

$$\langle u_n(1)|\rho(1)|u'_n(1)\rangle = \sum_p (\langle u_n(1)|\langle v_p(2)|)\rho(|u'_n(1)\rangle|v_p(2)\rangle) \tag{3.40}$$

By definition, $\rho(1)$ is obtained from ρ by performing a partial trace over (2):

$$\rho(1) = Tr_2\rho \tag{3.41}$$

Similarly, the operator:

$$\rho(2) = Tr_1\rho \tag{3.42}$$

has matrix elements

$$\langle v_p(2)|\rho(2)|v'_p(2)\rangle = \sum_n (\langle u_n(1)|\langle v_p(2)|)\rho(|u_n(1)\rangle|v'_p(2)\rangle) \tag{3.43}$$

It is clear why these operations are called partial traces. Moreover, we have:

$$Tr\rho = Tr_1(Tr_2\rho) = Tr_2(Tr_1\rho) \tag{3.44}$$

$\rho(1)$ and $\rho(2)$ are therefore, like ρ, operators whose trace is equal to 1. In particular, by recalling the definition (3.36) of single-particle density matrix, one can show that it respects the peculiarity to have trace equal to one. In fact:

$$\begin{aligned}
\sum_\alpha \rho^{sp}_{\alpha\alpha} &= \langle\Psi(\mathbf{r},t)|\hat{c}^\dagger_\alpha\hat{c}_\alpha|\Psi(\mathbf{r},t)\rangle \\
&= \langle\Psi(\mathbf{r},t)|\int d\mathbf{r}'d\mathbf{r}''\delta(\mathbf{r}'-\mathbf{r}'')\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}'')|\Psi(\mathbf{r},t)\rangle \\
&= \langle\Psi(\mathbf{r},t)|\int d\mathbf{r}'\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')|\Psi(\mathbf{r},t)\rangle \\
&= \langle\Psi(\mathbf{r},t)|\Psi(\mathbf{r},t)\rangle \\
&= 1
\end{aligned}$$

Then, it can be verified from their definitions that they are Hermitian.

Now let $A(1)$ be an observable acting over $\mathcal{E}(1)$ and $\widetilde{A}(1) \equiv A(1) \otimes \mathbb{1}(2)$, its extension in $\mathcal{E}$[3]. We obtain, using the definition of mean value (for simplicity, let us suppose to be in a pure system):

$$\begin{aligned}
\langle\widetilde{A}(1)\rangle &= Tr[\rho\widetilde{A}(1)] \\
&= \sum_{np}\sum_{n'p'}(\langle u_n(1)|\langle v_p(2)|)\rho(|u'_n(1)\rangle|v'_p(2)\rangle)(\langle u'_n(1)|\langle v'_p(2)|)A(1)\otimes\infty(2)(|u_n(1)\rangle|v_p(2)\rangle) \\
&= \sum_{np}\sum_{n'p'}(\langle u_n(1)|\langle v_p(2)|)\rho(|u'_n(1)\rangle|v'_p(2)\rangle)\langle u'_n(1)|A(1)|u_n(1)\rangle\langle v'_p(2)|v_p(2)\rangle \\
&= \sum_{nn'}\left[\sum_p(\langle u_n(1)|\langle v_p(2)|)\rho(|u'_n(1)\rangle|v_p(2)\rangle)\right]\langle u'_n(1)|A(1)|u_n(1)\rangle \\
&= \sum_{nn'}\langle u_n(1)|\rho(1)|u'_n(1)\rangle\langle u'_n(1)|A(1)|u_n(1)\rangle \\
&= \sum_n\langle u_n(1)|\rho(1)A(1)|u_n(1)\rangle \\
&= Tr_1[\rho(1)A(1)] \qquad (3.45)
\end{aligned}$$

---

[3] Given a linear operator $A(1)$ defined in $\mathcal{E}(1)$, we associate to it a linear operator $\widetilde{A}(1)$ acting on $\mathcal{E}$, which we call *extension of* $A(1)$ *in* $\mathcal{E}$, and which is characterized as follows: when $\widetilde{A}(1)$ is applied to a tensor product vector $|\varphi(1)\rangle \otimes |\chi(2)\rangle$, one obtains, by definition:

$$\widetilde{A}(1)[|\varphi(1)\rangle \otimes |\chi(2)\rangle] = [A(1)|\varphi(1)\rangle] \otimes |\chi(2)\rangle$$

We see that the partial trace $\rho(1)$ enables us to calculate all the mean values $\langle \widetilde{A}(1) \rangle$ as if the system (1) was isolated and had $\rho(1)$ as density operator.

The above results clearly show that the density operator can play a very crucial role in our physical predictions. In fact we know that it is impossible to assign a state vector to system (1) [or (2)] when the state of the global system (1) + (2) is not a product state. We now see that the density operator is a mathematical instrument much simpler than the state vector. In all cases (whether the global system is in a product state or not, whether it corresponds to a pure case or to a statistical mixture), one can always, thanks to the partial trace operation, assign a density operator to subsystem (1) [or (2)]. This allows to calculate all the physical predictions about such subsystem.

3.2.3 Semiconductor Bloch Equations (SBE)

Thanks to the definition of the single-particle density matrix

$$\rho^{sp}_{\alpha\beta} = \overline{\langle \hat{c}^\dagger_\alpha \hat{c}_\beta \rangle} \tag{3.46}$$

one can proceed in attempting to obtain the analogous equation, for the single density matrix, of the Liouville equation seen in (3.23) that, as we know, dictates the time evolution of the global density matrix.

Within the Schrödinger representation[4]:

$$\begin{aligned} i\hbar \frac{\partial \rho^{sp}_{\beta\alpha}}{\partial t} = i\hbar \frac{\partial \langle \hat{c}^\dagger_\alpha \hat{c}_\beta \rangle}{\partial t} = i\hbar \frac{\partial \langle \Psi(\mathbf{r},t) | \hat{c}^\dagger_\alpha \hat{c}_\beta | \Psi(\mathbf{r},t) \rangle}{\partial t} = \\ = i\hbar \int d\mathbf{r} \left[\frac{\partial}{\partial t} \Psi^*(\mathbf{r},t) \hat{c}^\dagger_\alpha \hat{c}_\beta \Psi(\mathbf{r},t) + \Psi^*(\mathbf{r},t) \hat{c}^\dagger_\alpha \hat{c}_\beta \frac{\partial}{\partial t} \Psi(\mathbf{r},t) + \right. \\ \left. \Psi^*(\mathbf{r},t) \frac{\partial}{\partial t} \hat{c}^\dagger_\alpha \hat{c}_\beta \Psi(\mathbf{r},t) + \Psi^*(\mathbf{r},t) \hat{c}^\dagger_\alpha \frac{\partial}{\partial t} \hat{c}_\beta \Psi(\mathbf{r},t) \right] \end{aligned} \tag{3.47}$$

---

[4] Obviously the result can be obtained in any representation. For example, the Heisenberg representation can provide the same result simply by starting from the Heisenberg equation for the field operator $\hat{\psi}$.

Under the hypothesis that the second quantization operator $\hat{c}$ does not depend on time, namely that the basis ϕ_n is time-independent, the last two terms of the previous expression are equal to zero, and thus

$$i\hbar\frac{\partial\rho^{sp}_{\beta\alpha}}{\partial t} = \int d\mathbf{r}[-\Psi^*(\mathbf{r},t)H\hat{c}^\dagger_\alpha\hat{c}_\beta\Psi(\mathbf{r},t)+0] = -\langle\Psi|H\hat{c}^\dagger_\alpha c_\beta|\Psi\rangle + \langle\Psi|\hat{c}^\dagger_\alpha c_\beta H|\Psi\rangle \tag{3.48}$$

so that the final expression is

$$i\hbar\frac{\partial\rho^{sp}_{\beta\alpha}}{\partial t} = \langle[\hat{c}^\dagger_\alpha\hat{c}_\beta, H]\rangle \tag{3.49}$$

The above equation, describing the time evolution of the single-particle density matrix, is called *Semiconductor Bloch Equation.* To explicit it we need the exact form of the system Hamiltonian. In the section “Physical system” we have already treated the term H (at least the single-particle terms, since the many-body contributions will be either approximated by means of the $t_1 - t_2$ approximation or neglected), thus it is sufficient to substitute it in equation (3.47) to obtain the desired result. In particular, under specific approximations that involve the many-body terms (since the single-particle ones can be treated exactly), the dynamics for ρ^{sp} can be described by the next, formally simple, equation

$$\frac{\partial\rho^{sp}_{\alpha_1\alpha_2}}{\partial t} = \sum_{\alpha'_1\alpha'_2}\mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho_{\alpha'_1\alpha'_2} \tag{3.50}$$

where the effective Liouville operator

$$\mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = \frac{1}{i\hbar}(\epsilon_{\alpha_1}-\epsilon_{\alpha_2})\delta_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} + \Gamma_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \tag{3.51}$$

is the sum of two terms: coherent (i.e., scattering-free) single particle evolution (ϵ_α denoting the single-particle energy of state α) plus energy-relaxation/dephasing dynamics; The latter is described in terms of the scattering tensor Γ, whose explicit form, given in [9], involves the microscopic in- and out-scattering rates for the various interaction mechanisms considered.

Before proceeding in the description of open systems from a microscopic point of view, let us see a scheme that summarizes the different approaches used in the transport theory. It is shown in Fig. 3.1.

3.2.4 Open systems

The theoretical description presented so far is typical of a spatially "closed" system, i.e., defined over the whole coordinate space. However, this is not the case of interest for the study of ultrafast phenomena in mesoscopic quantum devices, where the electro-optical properties of the carrier subsystem are strongly influenced by the spatial boundaries with the external environment. In what follows we shall present a generalization of the density-matrix formulation discussed so far to systems with open boundaries.

To this aim, let us focus on the conduction electron only, whose single-particle properties are fully described by the density matrix ρ^{sp} introduced previously. As discussed above, its time evolution depends on the interaction mechanisms considered as well as on the approximation level used to derive the proper set of kinetic equations.

As we have seen, the equation of motion for the single-density matrix ρ^{sp} can be schematically written as

$$\frac{\partial \rho^{sp}_{\alpha_1\alpha_2}}{\partial t} = \sum_{\alpha'_1\alpha'_2} \mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \rho^{sp}_{\alpha'_1\alpha'_2} \tag{3.52}$$

A system with open boundaries requires a real-space description, which can be obtained in terms of the phase-space formulation of quantum mechanics originally proposed by Wigner [21]. Generally speaking, this corresponds to introduce the following unitary transformation u,

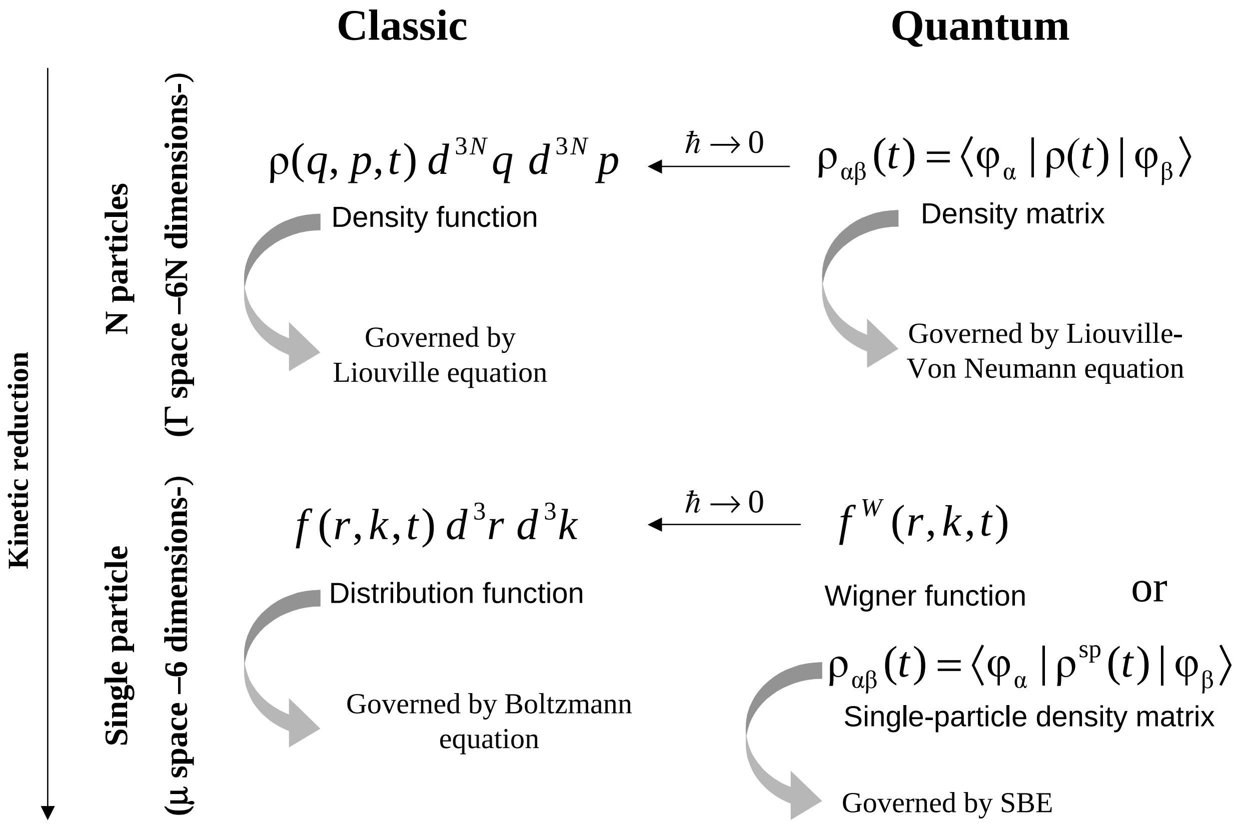

Figure 3.1: Schematic representation of the theoretical approaches, both in classical and in quantum theory, able to describe charge transport.

called Weyl-Wigner transformation[5], connecting the single-particle phase-space (α_1, α_2) to the desired (inasmuch as it contains the real-space coordinate) space-phase $(\mathbf{r}, \mathbf{k})$:

$$u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) = \Omega \int d\mathbf{r}' e^{-i\mathbf{k}\cdot\mathbf{r}'} \phi_{\alpha_1}\left(\mathbf{r} + \frac{\mathbf{r}'}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r} - \frac{\mathbf{r}'}{2}\right) \tag{3.53}$$

where ϕ are the electron single-particle wavefunctions. It can be regarded as the Fourier transform of the wavefunction autocorrelation with respect to the relative coordinate $\mathbf{r}'$. By applying the above Weyl-Wigner transform to the single-particle density matrix ρ^{sp}, we get

$$f^W(\mathbf{r}, \mathbf{k}) = \sum_{\alpha_1\alpha_2} \rho^{sp}_{\alpha_1\alpha_2} u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \tag{3.54}$$

The equation of motion for f^W can be obtained by applying the Weyl-Wigner transformation (3.53) to the kinetic equation (3.52). Thus, we get

$$\begin{aligned}
\frac{d}{dt} f^W(\mathbf{r}, \mathbf{k}) &= \sum_{\alpha_1\alpha_2} \frac{d\rho^{sp}_{\alpha_1\alpha_2}}{dt} u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \\
&= \sum_{\alpha_1\alpha_2} \left(\sum_{\alpha_1'\alpha_2'} \mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \rho^{sp}_{\alpha_1'\alpha_2'} \right) u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \\
&= \sum_{\alpha_1\alpha_2} u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \sum_{\alpha_1'\alpha_2'} \mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \rho^{sp}_{\alpha_1'\alpha_2'} \\
&= \sum_{\alpha_1\alpha_2} u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \sum_{\alpha_1'\alpha_2'} \mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \int d\mathbf{r}' d\mathbf{k}' u^*_{\alpha_1'\alpha_2'} f^W(\mathbf{r}', \mathbf{k}') \\
&= \int d\mathbf{r}' d\mathbf{k}' \mathcal{L}^W(\mathbf{r}, \mathbf{k}; \mathbf{r}', \mathbf{k}') f^W(\mathbf{r}', \mathbf{k}') \qquad (3.55)
\end{aligned}$$

where

$$\mathcal{L}^W(\mathbf{r}, \mathbf{k}; \mathbf{r}', \mathbf{k}') = \sum_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} u^*_{\alpha_1'\alpha_2'}(\mathbf{r}', \mathbf{k}') \tag{3.56}$$

is our Liouville operator in the new phase-space representation.

For a closed system, f^W is defined for any value of the real-space coordinate $\mathbf{r}$ and its time evolution is fully determined by its initial condition. In contrast, for a system with open

---

[5] See Appendix B

boundaries f^W is defined only[6] within a given region Ω of interest and its time evolution is dictated by the initial condition at t_0 inside such region, as well as by its values on the boundary $\mathbf{r}_b$ of the domain at any time $t' > t_0$. This boundary-condition scheme is usually referred to as "U scheme". The reason is motivated and explained in Fig. 3.2: More specifically, in order to properly impose the desired spatial boundary conditions, let us write Eq.(3.55) as

$$\begin{aligned}
\frac{d}{dt} f^W(\mathbf{r},\mathbf{k},t) &= \int d\mathbf{r}' d\mathbf{k}' \left[\mathcal{L}^W(\mathbf{r},\mathbf{k};\mathbf{r}'\mathbf{k}') - \left|\frac{\hbar\mathbf{k}}{m}\right| \delta(\mathbf{k}-\mathbf{k}')\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b)\right] f^W(\mathbf{r}',\mathbf{k}',t) + \\
&\quad \left|\frac{\hbar\mathbf{k}}{m}\right| \delta(\mathbf{r}-\mathbf{r}_b) f_b^W(\mathbf{k}) \\
&= \int d\mathbf{r}' d\mathbf{k}' \widetilde{\mathcal{L}}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}') f^W(\mathbf{r}',\mathbf{k}',t) + \widetilde{\mathcal{S}}^W(\mathbf{r},\mathbf{k}) \qquad (3.57)
\end{aligned}$$

with

$$\widetilde{\mathcal{S}}^W(\mathbf{r},\mathbf{k}) = |v(\mathbf{k})| f_b^W(\mathbf{k}) \delta(\mathbf{r}-\mathbf{r}_b) \qquad (3.58)$$

and

$$\widetilde{\mathcal{L}}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}') = \mathcal{L}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}') - |v(\mathbf{k})| \delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}') \qquad (3.59)$$

where $v(\mathbf{k})$ denotes the carrier group velocity normal to the boundary surface (i.e., we assume that $r_b = r_{left}$ and $r_b = r_{right}$ - in the hypothesis to be in one-dimensional system - respectively if $k > 0$ and $k < 0$) and $f^W(\mathbf{r}_b, \mathbf{k}, t) \equiv f_b^W(\mathbf{k})$ is the Wigner function describing the distribution of injected carriers. The equation (3.58) describes the source term, namely carrier injection from the boundaries into the simulated region.

Let us now discuss about the relation $f^W(\mathbf{r}_b, \mathbf{k}, t) \equiv f_b^W(\mathbf{k})$. The question is: "In stationary or steady-state conditions is it true that $f^W(\mathbf{r}_b, \mathbf{k}) \equiv f_b^W(\mathbf{k})$?". The answer is "yes".
To demonstrate this property, let us consider the equation (3.57). The latter can be rewritten as:

$$\frac{d}{dt} f^W(\mathbf{r},\mathbf{k},t) = \int d\mathbf{r}' d\mathbf{k}' \mathcal{L}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}') f^W(\mathbf{r}',\mathbf{k}',t) + \left|\frac{\hbar\mathbf{k}}{m}\right| [f_b^W(\mathbf{k}) - f^W(\mathbf{r},\mathbf{k},t)]\delta(\mathbf{r}-\mathbf{r}_b) \qquad (3.60)$$

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[6] In reality $f^W(\mathbf{r},\mathbf{k})$, as such, is mathematically defined over the whole phase-space μ; however, we impose that such function assumes a particular value on the boundaries, since we are not interested in its behaviour outside.

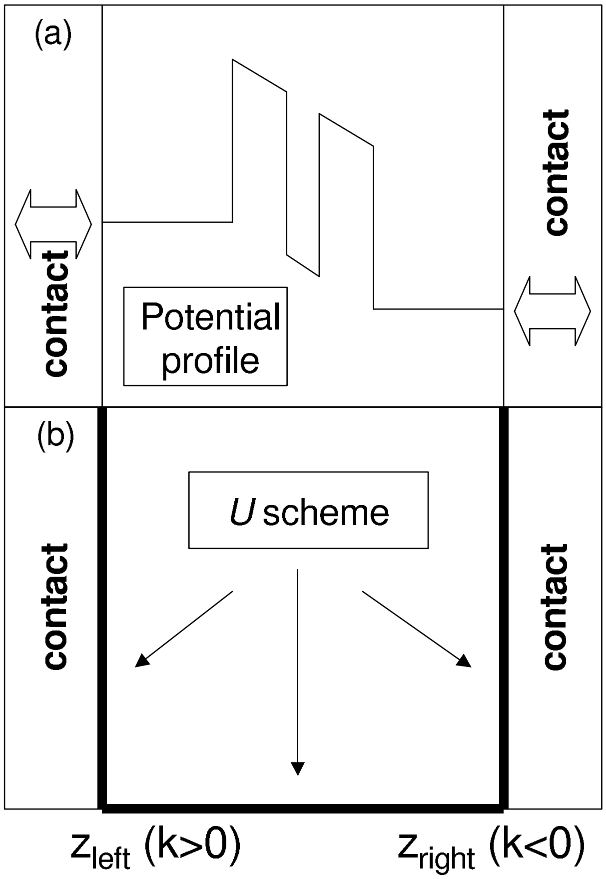

Figure 3.2: Schematic representation of the device active region sandwiched between its electrical contacts (a) and the corresponding **U** boundary-condition scheme for a one-dimensional system (b). The latter implies, in particular, the knowledge of the incoming Wigner function $f^W(z_b, k)$, i.e., $f^W(z_{left}, k > 0)$ and $f^W(z_{right}, k < 0)$.

By using the transformation $f^W(\mathbf{r},\mathbf{k},t) = \sum_{\alpha\beta} u_{\alpha\beta}(\mathbf{r},\mathbf{k})\rho_{\alpha\beta}(t)$, Eq.(3.60) becomes:

$$\begin{aligned}\sum_{\alpha\beta} u_{\alpha\beta}(\mathbf{r},\mathbf{k})\frac{d\rho^{sp}_{\alpha\beta}}{dt} &= \int d\mathbf{r}'d\mathbf{k}'\mathcal{L}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}')\sum_{\alpha'\beta'} u_{\alpha'\beta'}(\mathbf{r}',\mathbf{k}')\rho^{sp}_{\alpha'\beta'}(t) \\ &\quad +|v(\mathbf{k})|\left[f^W_b(\mathbf{k}) - f^W(\mathbf{r},\mathbf{k},t)\right]\delta(\mathbf{r}-\mathbf{r}_b)\end{aligned}$$

i.e.,

$$\begin{aligned}\sum_{\alpha\beta}\int d\mathbf{r}d\mathbf{k}u_{\alpha\beta}(\mathbf{r},\mathbf{k})u^*_{\alpha''\beta''}(\mathbf{r},\mathbf{k})\frac{d}{dt}\rho^{sp}_{\alpha\beta}(t) = \\ \sum_{\alpha'\beta'}\int d\mathbf{r}'d\mathbf{k}'d\mathbf{r}d\mathbf{k}\;\mathcal{L}^W(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}')u_{\alpha'\beta'}(\mathbf{r}',\mathbf{k}')u^*_{\alpha''\beta''}(\mathbf{r},\mathbf{k})\rho^{sp}_{\alpha'\beta'}(t) + \\ \int d\mathbf{r}d\mathbf{k}u^*_{\alpha''\beta''}(\mathbf{r},\mathbf{k})|v(\mathbf{k})|\left[f^W_b(\mathbf{k}) - f^W(\mathbf{r},\mathbf{k},t)\right]\delta(\mathbf{r}-\mathbf{r}_b)\end{aligned} \tag{3.61}$$

By considering the property

$$\int d\mathbf{r}d\mathbf{k}u_{\alpha\beta}(\mathbf{r},\mathbf{k})u^*_{\alpha''\beta''}(\mathbf{r},\mathbf{k}) = \delta_{\alpha\alpha''}\delta_{\beta\beta''},$$

Eq.(3.61) becomes:

$$\frac{d}{dt}\rho^{sp}_{\alpha''\beta''}(t) = \sum_{\alpha'\beta'}\mathcal{L}_{\alpha'\beta',\alpha''\beta''}\rho^{sp}_{\alpha'\beta'}(t) + \int d\mathbf{r}d\mathbf{k}\;u^*_{\alpha''\beta''}(\mathbf{r},\mathbf{k})|v(\mathbf{k})|\left[f^W_b(\mathbf{k}) - f^W(\mathbf{r},\mathbf{k},t)\right]\delta(\mathbf{r}-\mathbf{r}_b)$$

Let us suppose that the basis states $\{\alpha\}$ diagonalize ρ^{sp}, that is $\rho^{sp}_{\alpha\beta} = \rho^{sp}_{\alpha\alpha}\delta_{\alpha\beta}$; in this case we obtain:

$$\begin{aligned}\frac{d}{dt}\rho^{sp}_{\alpha\alpha}(t) &= \sum_{\alpha'}\mathcal{L}_{\alpha\alpha,\alpha'\alpha'}\rho^{sp}_{\alpha'\alpha'} + \int d\mathbf{r}d\mathbf{k}\;u^*_{\alpha\alpha}(\mathbf{r},\mathbf{k})|v(\mathbf{k})|\left[f^W_b(\mathbf{k}) - f^W(\mathbf{r},\mathbf{k},t)\right]\delta(\mathbf{r}-\mathbf{r}_b) \\ &= \sum_{\alpha'}\mathcal{L}^W_{\alpha\alpha,\alpha'\alpha'}\rho^{sp}_{\alpha'\alpha'} + \int d\mathbf{k}\;u^*_{\alpha\alpha}(\mathbf{r}_b,\mathbf{k})|v(\mathbf{k})|\left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b,\mathbf{k},t)\right]\end{aligned}$$

Finally, by means of Eq.(3.51), the above equation in stationary regime reduces to:

$$-\sum_{\alpha'} \Gamma_{\alpha\alpha,\alpha'\alpha'} \rho^{sp}_{\alpha'\alpha'} + \int d\mathbf{k}\; u^*_{\alpha\alpha}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| \left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right] = 0 \tag{3.62}$$

Now, in the scattering/dephasing-free case ($\Gamma = 0$) Eq. (3.62) becomes:

$$\int d\mathbf{k}\; u^*_{\alpha\alpha}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| \left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right] = 0, \quad \forall \alpha$$

i.e.,

$$f^W(\mathbf{r}_b, \mathbf{k}) = f^W_b(\mathbf{k})$$

This result tells us that, in the stationary and scattering/dephasing-freecase, the "incoming" Wigner function on our spatial boundaries is equal to the thermal distribution entering the source term. Now, the point is what happens for Γ different from zero.
To answer this question, let us consider that the scattering superoperator Γ, as such, preserves the total number of particles inside the simulated region, i.e., the trace of the density matrix is not affected by scattering/dephasing. It follows that, by summing on α Eq. (3.62), we get:

$$\begin{aligned}
0 &= -\sum_\alpha \sum_{\alpha'} \Gamma_{\alpha\alpha,\alpha'\alpha'} \rho^{sp}_{\alpha'\alpha'} + \sum_\alpha \int d\mathbf{k}\; u^*_{\alpha\alpha}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| \left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right] \\
&= \int d\mathbf{k}\; \sum_\alpha u^*_{\alpha\alpha}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| \left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right] \\
&= \int d\mathbf{k}\; \sum_\alpha |v(\mathbf{k})| \left[f^W_b(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right]
\end{aligned} \tag{3.63}$$

where we have employed the following relations:

$$\sum_{\alpha\alpha'} \Gamma_{\alpha\alpha,\alpha'\alpha'} \rho^{sp}_{\alpha'\alpha'} = 0$$

which follows from the hypothesis that the scattering does not change the number of particles, and

$$\sum_\alpha u^*_{\alpha\alpha}(\mathbf{r}, \mathbf{k}) = 1, \quad \forall\, \mathbf{r}$$

Therefore, as for the scattering/dephasing-free case, Eq. (3.63) tells us that:

$$f^W(\mathbf{r}_b, \mathbf{k}) = f_b^W(\mathbf{k})$$

Let us finally consider the case in which, due e.g. to electron-hole recombination processes, the number of particles within the simulated region is not conserved. In this case, Eq. (3.62) becomes:

$$0 = -\sum_{\alpha}\sum_{\alpha'} \Gamma_{\alpha\alpha,\alpha'\alpha'} \rho^{sp}_{\alpha'\alpha'} + \sum_{\alpha} \int d\mathbf{k}\; u^*_{\alpha\alpha}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| \left[f_b^W(\mathbf{k}) - f^W(\mathbf{r}_b, \mathbf{k}) \right]$$

where, contrary to the previous situation, $\sum_{\alpha\alpha'} \Gamma_{\alpha\alpha,\alpha'\alpha'} \rho^{sp}_{\alpha'\alpha'}$ is different from zero. It is clear that this new condition implies that the value of the Wigner function on the system boundary is renormalized by the scattering term Γ. This confirms the idea (Frensley 1990) that the effect of scattering inside the device is equivalent to that of spatial boundaries, and vice versa.

Given the above Wigner formulation for open systems, we now go back to the density-matrix description via the following Weyl-Wigner transform

$$\rho^{sp}_{\alpha_1\alpha_2} = \int d\mathbf{r} d\mathbf{k} u^*_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) f^W(\mathbf{r}, \mathbf{k}) \tag{3.64}$$

By applying the above inverse transformation to Eq.(3.57), we finally obtain:

$$\frac{d}{dt} \rho^{sp}_{\alpha_1\alpha_2} = \sum_{\alpha'_1\alpha'_2} \widetilde{\mathcal{L}}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \rho^{sp}_{\alpha'_1\alpha'_2} + \widetilde{\mathcal{S}}_{\alpha_1\alpha_2} \tag{3.65}$$

where

$$\widetilde{\mathcal{L}}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = \mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} + \Delta\mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \tag{3.66}$$

is the Liouville operator in Eq.(3.52) renormalized by the quantity

$$\Delta\mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = -\int d\mathbf{r}_b d\mathbf{k} u^*_{\alpha_1\alpha_2}(\mathbf{r}_b, \mathbf{k}) |v(\mathbf{k})| u_{\alpha'_1\alpha'_2}(\mathbf{r}_b, \mathbf{k}) \tag{3.67}$$

while

$$\widetilde{\mathcal{S}}_{\alpha_1\alpha_2} = \int d\mathbf{r} d\mathbf{k} u^*_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) \widetilde{\mathcal{S}}^W(\mathbf{r}, \mathbf{k}) \tag{3.68}$$

is the source term in Eq.(3.58) written in the density-matrix representation.

Equation (3.65) is the desired generalization to the case of systems with open boundaries of the conventional dynamical equation (3.52). In addition to the source term described in Eq.(3.68), the presence of boundary conditions induces modifications to the Liouville operator $\mathcal{L}$. In particular, the open character of the system results in a non-Hermitian correction $\Delta\mathcal{L}$ to the Liouville operator $\mathcal{L}$, whose effect is equivalent to a purely dissipative process within the simulated region Ω, as originally pointed out in [5].

Since our aim is to study the carrier dynamics only within the simulated region Ω, given any physical single-particle quantity A, its average value is given by

$$\langle A\rangle = \int_\Omega d\mathbf{r}\int d\mathbf{k} f^W(\mathbf{r},\mathbf{k})A^W(\mathbf{r},\mathbf{k}) \tag{3.69}$$

where A^W denotes the operator A in our Weyl-Wigner representation (see appendix B). However, this equation involves the whole phase-space μ. Since we want to treat open quantum devices, i.e., systems with finite spatial dimensions, it is useful to rewrite the previous equation such to involve the simulated region Ω only. Indeed, it is possible to show that

$$\langle A\rangle = \int_\Omega d\mathbf{r}\int d\mathbf{k} \breve{f}^W(\mathbf{r},\mathbf{k})A^W(\mathbf{r},\mathbf{k}) \tag{3.70}$$

where $\breve{f}^W$ is the Wigner function defined only inside the region Ω. To show the equivalence between Eq.(3.69) and Eq.(3.70), one proceeds as follows. By using the inverse of Eq.(3.64) and the relation $u_{\alpha\beta} = u^*_{\beta\alpha}$, Eq. (3.69) becomes:

$$\begin{aligned}
\int_\Omega d\mathbf{r}\int d\mathbf{k} f^W(\mathbf{r},\mathbf{k})A^W(\mathbf{r},\mathbf{k}) &= \int_\Omega d\mathbf{r}\int d\mathbf{k} \sum_{\alpha_1\alpha_2}\rho^{sp}_{\alpha_1\alpha_2}u_{\alpha_1\alpha_2}(\mathbf{r},\mathbf{k})\sum_{\alpha'_1\alpha'_2}A_{\alpha'_2\alpha'_1}u_{\alpha'_2\alpha'_1}(\mathbf{r},\mathbf{k}) \\
&= \sum_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho^{sp}_{\alpha_1\alpha_2}A_{\alpha'_2\alpha'_1}\int_\Omega d\mathbf{r}\int d\mathbf{k} u_{\alpha_1\alpha_2}(\mathbf{r},\mathbf{k})u^*_{\alpha'_1\alpha'_2}(\mathbf{r},\mathbf{k}) \\
&= \sum_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho^{sp}_{\alpha_1\alpha_2}A_{\alpha'_2\alpha'_1}\mathcal{U}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \\
&= \sum_{\alpha'_1\alpha'_2}\left[\sum_{\alpha_1\alpha_2}\rho^{sp}_{\alpha_1\alpha_2}\mathcal{U}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\right]A_{\alpha'_2\alpha'_1} \\
&= \sum_{\alpha'_1\alpha'_2}\breve{\rho}^{sp}_{\alpha'_1\alpha'_2}A_{\alpha'_2\alpha'_1} \\
&= Tr\left(\breve{\rho}^{sp}A\right)
\end{aligned} \tag{3.71}$$

where $\mathcal{U}$ can be regarded as a projector operator acting on our simulated region Ω. Its projector nature can be easily verified by showing that applying the operator $\mathcal{U}$ once or twice to a generic Weyl-Wigner quantity, we get the same result. More specifically,

$$\breve{\rho}^{sp}_{\alpha\beta} = \sum_{\alpha'\beta'} \mathcal{U}_{\alpha\beta,\alpha'\beta'} \breve{\rho}^{sp}_{\alpha'\beta'} \tag{3.72}$$

In fact:

$$\begin{aligned}
\sum_{\alpha'\beta'} \mathcal{U}_{\alpha\beta,\alpha'\beta'} \breve{\rho}^{sp}_{\alpha'\beta'} &= \sum_{\alpha'\beta',\alpha''\beta''} \mathcal{U}_{\alpha\beta,\alpha'\beta'} \mathcal{U}_{\alpha'\beta',\alpha''\beta''} \rho^{sp}_{\alpha''\beta''} \\
&= \sum_{\alpha'\beta',\alpha''\beta''} \int_\Omega d\mathbf{r}' d\mathbf{k}' u^*_{\alpha\beta}(\mathbf{r}',\mathbf{k}') u_{\alpha'\beta'}(\mathbf{r}',\mathbf{k}') \int_\Omega d\mathbf{r}'' d\mathbf{k}'' u^*_{\alpha'\beta'}(\mathbf{r}'',\mathbf{k}'') u_{\alpha''\beta''}(\mathbf{r}'',\mathbf{k}'') \rho^{sp}_{\alpha''\beta''} \\
&= \sum_{\alpha''\beta''} \int_\Omega d\mathbf{r}' d\mathbf{k}' d\mathbf{r}'' d\mathbf{k}'' u^*_{\alpha\beta}(\mathbf{r}',\mathbf{k}') u_{\alpha''\beta''}(\mathbf{r}'',\mathbf{k}'') \delta(\mathbf{r}'-\mathbf{r}'') \delta(\mathbf{k}'-\mathbf{k}'') \rho^{sp}_{\alpha''\beta''} \\
&= \sum_{\alpha''\beta''} \int_\Omega d\mathbf{r}' d\mathbf{k}' u^*_{\alpha\beta}(\mathbf{r}',\mathbf{k}') u_{\alpha''\beta''}(\mathbf{r}',\mathbf{k}') \rho^{sp}_{\alpha''\beta''} \\
&= \sum_{\alpha''\beta''} \mathcal{U}_{\alpha\beta,\alpha''\beta''} \rho^{sp}_{\alpha''\beta''} \\
&= \breve{\rho}^{sp}_{\alpha\beta}
\end{aligned} \tag{3.73}$$

We stress that when Ω coincides with *all* the μ-space, the quantity $\mathcal{U}$ becomes a Dirac delta function, namely the system is projected on itself, that means that the space of interest is the whole phase-space.

Coming back to the equivalence between Eq.(3.69) and Eq.(3.70), let us consider again the second one:

$$\begin{aligned}
\langle A \rangle &= \int_\Omega d\mathbf{r} \int d\mathbf{k} \breve{f}^W(\mathbf{r},\mathbf{k}) A^W(\mathbf{r},\mathbf{k}) \\
&= \int_\Omega d\mathbf{r} \int d\mathbf{k} \sum_{\alpha\beta} \breve{\rho}^{sp}_{\alpha\beta} u_{\alpha\beta}(\mathbf{r},\mathbf{k}) \sum_{\alpha'\beta'} A_{\beta'\alpha'} u_{\alpha'\beta'}(\mathbf{r},\mathbf{k}) \\
&= \sum_{\alpha\beta,\alpha'\beta'} \breve{\rho}^{sp}_{\alpha\beta} A_{\beta'\alpha'} \int_\Omega d\mathbf{r} \int d\mathbf{k} u_{\alpha\beta}(\mathbf{r},\mathbf{k}) u_{\alpha'\beta'}(\mathbf{r},\mathbf{k}) \\
&= \sum_{\alpha\beta,\alpha'\beta'} \breve{\rho}^{sp}_{\alpha\beta} A_{\beta'\alpha'} \mathcal{U}_{\alpha\beta,\alpha'\beta'} \\
&= \sum_{\alpha'\beta'} \left[\sum_{\alpha\beta} \breve{\rho}^{sp}_{\alpha\beta} \mathcal{U}_{\alpha\beta,\alpha'\beta'} \right] A_{\beta'\alpha'}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{\alpha'\beta'} \rho^{sp}_{\alpha'\beta'} A_{\beta'\alpha'} \\
&= Tr\left(\breve{\rho}^{sp} A\right) \qquad (3.74)
\end{aligned}
$$

This is exactly the same expression written in Eq. (3.71) and thus the equivalence is shown. Equation (3.74) tells us that the evaluation of average quantities requires the knowledge of the operator $\mathcal{U}$.

Obviously such approach applies to any observable A, that means that we can obtain macroscopic quantities simply from the knowledge of the Wigner function inside the device.

3.2.5 Failure of the "canonical" Wigner function formalism

Although the above theoretical approach seems appropriate, at least formally, to describe adequately open systems, in what follows we shall see that the Wigner-function formalism analyzed so far presents serious intrinsic limitations when applied to the study of charge transport in open quantum devices. To overcome such limitations, we shall introduce a new approach, called "Generalized Wigner function". Before discussing such generalized scheme, let us consider a prototypical example which clearly shows that the canonical Wigner-function approach introduced so far does not work properly. To this end , let us focus on a very simple semiconductor nanostructure: a single-barrier equidistant from the device contacts (see Fig. 3.3). Here, as basis states α we adopt the scattering states of the device potential profile; moreover, to better identify the role played by carrier injection, we shall neglect all other sources of energy relaxation/dephasing in the device active region, like carrier-phonon and carrier-carrier scattering: $\Gamma_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = 0$ [see Eq.(3.51)]. Under these assumptions, Eq.(3.65) in steady-state conditions reduces to:

$$
\frac{1}{i\hbar}(\epsilon_{\alpha_1} - \epsilon_{\alpha_2})\rho^{sp}_{\alpha_1\alpha_2} + \sum_{\alpha'_1\alpha'_2} \Delta\mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho^{sp}_{\alpha'_1\alpha'_2} + \tilde{\mathcal{S}}_{\alpha_1\alpha_2} = 0 \qquad (3.75)
$$

To fully identify the non-physical nature of the results obtained within the present Wigner-function approach, we have compared them to those obtained by a Boltzmann-like phenomenological model, i.e., a model where the scattering is Boltzmann-like and the open character is

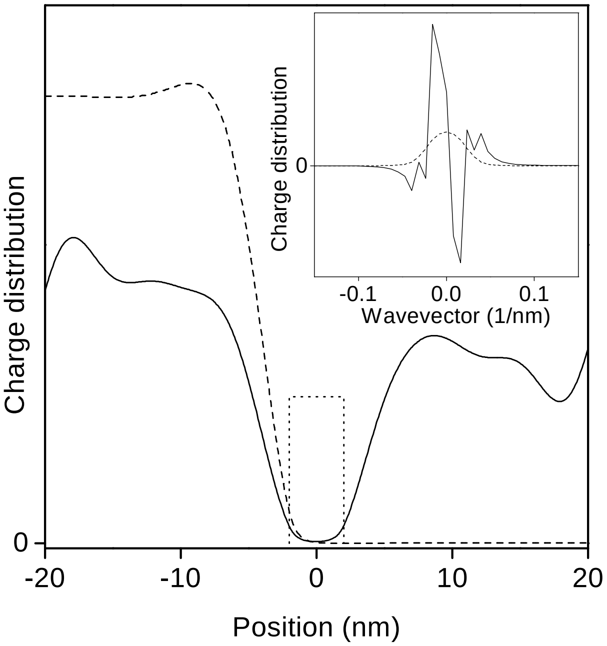

Figure 3.3: Comparison between the real-space charge distribution obtained from the phenomenological injection model in Eq.(3.76) [$n(\mathbf{r}) = \sum_\alpha f_\alpha |\phi_\alpha(\mathbf{r})|^2$ - dashed curve] and the microscopic model in Eq.(3.75) [$n(\mathbf{r}) = \sum_{\alpha_1\alpha_2} \rho^{sp}_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r}) \phi^*_{\alpha_2}(\mathbf{r})$ - solid curve] for a GaAs-based single barrier structure (height $V_0 = 0.5eV$ and width $a = 4nm$) equidistant from the electrical contacts. In this room-temperature simulation, due to a misalignment $\Delta\mu = 0.2eV$ of the left and right chemical potential, carriers are primarily injected from left. The corresponding charge distribution in momentum space is also reported in the inset.

treated via a phenomenological relaxation-time-like term:

$$\frac{d}{dt} f_\alpha = \sum_{\alpha'} (f_{\alpha'} W_{\alpha'\alpha} - f_\alpha W_{\alpha\alpha'}) + \frac{f^b_\alpha - f_\alpha}{\tau_\alpha} \tag{3.76}$$

where f_α represents the single-particle carrier distribution over the electronic states α of the device, $W_{\alpha\alpha'}$ the microscopic scattering rates (due, i.e., to carrier-carrier and carrier-phonon interaction), f^b_α denotes the equilibrium carrier distribution in the contacts and τ_α can be regarded as the device transit time for an electron in state α. Thus, the last term describes carrier injection/loss on a partially phenomenological level and does not depend on the real position of the device spatial boundaries.

Figure 3.3 refers to a single-barrier potential profile where carriers are primarily injected from left. Here, the simulated real-space charge distribution obtained from the phenomenological injection model in Eq.(3.76) (dashed curve) is compared to that of the microscopic model in (3.75) (solid curve). As we can see, the two models give completely different results. The phenomenological model gives basically what we expected: since we have significant carrier injection from left only and since the potential barrier is relatively high, the carrier distribution is mainly located on the left side. In contrast, the microscopic model gives an almost symmetric charge distribution. In order to understand the origin of this unphysical result, let us focus on the nature of the Wigner-Weyl transform (3.53), rewritten as

$$u_{\alpha_1\alpha_2}(\mathbf{r}, \mathbf{k}) = \Omega \int d\mathbf{r}' e^{-i\mathbf{k}\cdot\mathbf{r}'} \phi_{\alpha_1}\left(\mathbf{r} + \frac{\mathbf{r}'}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r} - \frac{\mathbf{r}'}{2}\right)$$

The generic scattering state α on the left comes out to be an almost equally weighted superposition of $+k$ and $-k$: $\phi_\alpha(z) = a_k e^{ikz} + b_k e^{-ikz}$ (we have considered the one-dimensional case). This, in turn, means that the generic plane-wave state k injected from left contact is also an almost[7] equally weighted superposition of the left and right scattering states. This is the reason why the charge distribution (solid curve in Fig.3.3) is almost symmetric: any electron injected

---

[7] In the limit $a_k \to b_k$ (i.e., when the barrier produces a full reflection, namely the transmission coefficient is equal to zero), the carrier distribution becomes completely symmetric.

from left couples to left as well as to right scattering states. The anomaly of the microscopic model is even more pronounced if we look at the carrier distribution in momentum space (see inset in Fig.3.3). While for the phenomenological model (dashed curve) we get a positive-definite distribution showing, as expected, the two symmetric wavevector components of the scattering state, the microscopic result is not positive definite; this tells us that the boundary-condition scheme considered so far does not provide a "good" Wigner function.

Beside that, another significant physical inconsistency comes out by observing the form of the source term. Contrary to the phenomenological injection/loss term in (3.76), the microscopic injection is intrinsically non-diagonal, i.e., the injection of a carrier with well-defined wavevector $\mathbf{k}$ [see Eq.(3.58)] is described by a non-diagonal source contribution $\widetilde{\mathcal{S}}_{\alpha_1\alpha_2}$. In other words, *we inject into the device active region a coherent superposition of states* α_1 *and* α_2, in clear contrast with the idea of injection from a thermal -i.e. diagonal- charge reservoir. To try to overcome this problem still within the canonical Wigner representation, i.e., in order to identify a source term $\widetilde{\mathcal{S}}(\mathbf{r},\mathbf{k})$ corresponding to a diagonal source term within the α-representation, it is easy to realize that this would require to adopt a non-local (in space) source term. Indeed, we have:

$$\widetilde{\mathcal{S}}_{\alpha_1\alpha_2} = \int d\mathbf{r} d\mathbf{k} u^*_{\alpha_1\alpha_2} \widetilde{\mathcal{S}}^W(\mathbf{r},\mathbf{k}) \qquad (3.77)$$

By inverting Eq.(3.77) and imposing a diagonal form of the source term ($\widetilde{\mathcal{S}}_{\alpha_1\alpha_2} = \widetilde{\mathcal{S}}_{\alpha_1\alpha_1}\delta_{\alpha_1\alpha_2}$), we get:

$$\widetilde{\mathcal{S}}^W(\mathbf{r},\mathbf{k}) = \sum_\alpha \widetilde{\mathcal{S}}_{\alpha\alpha} u_{\alpha\alpha}(\mathbf{r},\mathbf{k}) \qquad (3.78)$$

The above source function can never be point-like in space, as requested by our boundary-condition scheme (see Fig.3.2).

The scenario previously discussed is highly non-physical; it can be ascribed to the boundary-condition scheme employed so far, which implies injection of planewave electrons, regardless of the device potential profile. This is an intrinsic limitation of the conventional Wigner-function representation $\mathbf{r},\mathbf{k}$. It is then clear that, in order to overcome the serious limitations previously discussed, what we need is a *new boundary-condition scheme realizing also diagonal injection* *over the scattering states α of the device potential profile.* For these reasons we are going to show how to develop the new scheme, called "Generalized Wigner function approach".

3.2.6 Generalized Wigner-function approach

The key idea is to extend the Weyl-Wigner transform in (3.53) from the $\mathbf{k}$ to a generic basic set $\{|\beta\rangle\}$. Thus, by using the basis functions $\chi_\beta(\mathbf{r})$ that, in general, are different from the basis functions $\phi_\alpha(\mathbf{r})$, it is possible to define a new Weyl-Wigner transform (Generalized Transform)

$$u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) = \Omega \int d\mathbf{r}' \phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \chi^*_{\beta_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \chi_{\beta_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \tag{3.79}$$

where Ω denotes again the volume of the simulated region and "G" stays for "Generalized". Such equation does not represent a unitary transformation corresponding to a simple basis change; it amounts to a non-trivial projection operator involving the real space Wigner coordinate $\mathbf{r}$:

$$u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) = \langle\beta_1|\alpha_1\rangle|\mathbf{r}\rangle\langle\mathbf{r}|\langle\alpha_2|\beta_2\rangle \tag{3.80}$$

Let us now show where Eq.(3.80) comes from. We define

$$\begin{aligned} u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2} &\equiv \langle\beta_1|\alpha_1\rangle\langle\alpha_2|\beta_2\rangle \\ &= \int d\mathbf{r_1} d\mathbf{r_2} \langle\beta_1|\mathbf{r_1}\rangle\langle\mathbf{r_1}|\alpha_1\rangle\langle\alpha_2|\mathbf{r_2}\rangle\langle\mathbf{r_2}|\beta_2\rangle \\ &= \int d\mathbf{r_1} d\mathbf{r_2} \chi^*_{\beta_1}(\mathbf{r_1})\phi_{\alpha_1}(\mathbf{r_1})\phi^*_{\alpha_2}(\mathbf{r_2})\chi_{\beta_2}(\mathbf{r_2}) \\ &= \int d\mathbf{r} d\mathbf{r}' \phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \chi^*_{\beta_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \chi_{\beta_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \\ &= \int d\mathbf{r} u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) \end{aligned} \tag{3.81}$$

where $\mathbf{r}' = \mathbf{r_1} - \mathbf{r_2}$ and $\mathbf{r} = (\mathbf{r_1} + \mathbf{r_2})/2$.

The reasons that lead to consider $u^{WG}(\mathbf{r})$ as a projector, comes from the observation that by integrating it on the *whole* real space we obtain a Dirac delta function. Moreover, we shall show (see below) that by applying the $u^{WG}(\mathbf{r})$ once or twice to a density matrix, we get the same result. It is important to stress that if we take as basis functions χ ordinary plane waves, i.e.,

$$\chi_\beta\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)=e^{-i\mathbf{k}_\beta\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)}$$

we obtain exactly the usual Weyl-Wigner transform defined in (3.53). This is why Eq.(3.79) is called "Generalized Weyl-Wigner transform".

In analogy to (3.54), the generalized Wigner function[8] is given by

$$f^{WG}_{\beta_1\beta_2}(\mathbf{r})=\sum_{\alpha_1\alpha_2}\rho^{sp}_{\alpha_1\alpha_2}u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) \tag{3.82}$$

It can be shown that this equation is well defined inasmuch as, under the hypothesis that the basis $\{\chi\}$ and $\{\phi\}$ coincide, we have

$$\sum_\beta f^{WG}_{\beta\beta}(\mathbf{r},t)=|\Psi(\mathbf{r},t)|^2$$

which agrees with the properties of the usual Weyl-Wigner approach[9] [see Eq.(**??**)]. In fact:

$$\sum_\beta f^{WG}_{\beta\beta}(\mathbf{r}) \quad = \quad \sum_\beta\sum_{\alpha_1\alpha_2}\rho^{sp}_{\alpha_1\alpha_2}u^{WG}_{\alpha_1\alpha_2,\beta\beta}(\mathbf{r})$$

---

[8] Starting from equation (3.82) we can demonstrate that the quantity $u^{WG}(\mathbf{r})$ is a projector, i.e.,

$$\sum_{\alpha_1'\alpha_2'}u^{WG}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}(\mathbf{r})\rho^{sp}_{\alpha_1'\alpha_2'}=\sum_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''}u^{WG}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}(\mathbf{r})u^{WG}_{\alpha_1''\alpha_2'',\alpha_1'\alpha_2'}(\mathbf{r})\rho^{sp}_{\alpha_1'\alpha_2'}$$

Indeed, under the hypothesis that $\{\chi\}\equiv\{\phi\}$, we have

$$\begin{aligned}
\sum_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''} & u^{WG}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}(\mathbf{r}) \quad u^{WG}_{\alpha_1''\alpha_2'',\alpha_1'\alpha_2'}(\mathbf{r})\rho^{sp}_{\alpha_1'\alpha_2'}= \\
= & \sum_{\alpha_1'\alpha_2'}\rho^{sp}_{\alpha_1'\alpha_2'}\sum_{\alpha_1''\alpha_2''}\int d\mathbf{r}'\phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)\phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right)\phi^*_{\alpha_1''}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)\phi_{\alpha_2''}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \\
& \int d\mathbf{r}''\phi_{\alpha_1''}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right)\phi^*_{\alpha_2''}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right)\phi^*_{\alpha_1'}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right)\phi_{\alpha_2'}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right) \\
= & \sum_{\alpha_1'\alpha_2'}\rho^{sp}_{\alpha_1'\alpha_2'}\int d\mathbf{r}'\phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)\phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right)\phi^*_{\alpha_1'}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right)\phi_{\alpha_2'}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \\
= & \sum_{\alpha_1'\alpha_2'}\rho^{sp}_{\alpha_1'\alpha_2'}u^{WG}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}(\mathbf{r})
\end{aligned}$$

[9] Here, for the sake of simplicity, we have supposed to be in a pure state.

$$
\begin{aligned}
&= \sum_{\alpha_1\alpha_2} \rho^{sp}_{\alpha_1\alpha_2} \sum_{\beta} \int d\mathbf{r}' \phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \phi^*_{\beta}\left(\mathbf{r}+\frac{\mathbf{r}'}{2}\right) \phi_{\beta}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}'}{2}\right) \\
&= \sum_{\alpha_1\alpha_2} \rho^{sp}_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r}) \phi^*_{\alpha_2}(\mathbf{r}) \\
&= \sum_{\alpha_1\alpha_2} \langle \alpha_1|\Psi\rangle\langle\Psi|\alpha_2\rangle\langle\mathbf{r}|\alpha_1\rangle\langle\alpha_2|\mathbf{r}\rangle \\
&= |\Psi(\mathbf{r},t)|^2
\end{aligned}
\tag{3.83}
$$

By combining Eqs.(3.54) and (3.82), the Generalized Wigner function f^{WG} can be easily expressed in terms of the standard one as:

$$
f^{WG}_{\beta_1\beta_2}(\mathbf{r}) = \int d\mathbf{r}' d\mathbf{k}' \mathcal{K}_{\beta_1\beta_2}(\mathbf{r};\mathbf{r}',\mathbf{k}') f^W(\mathbf{r}',\mathbf{k}')
\tag{3.84}
$$

with

$$
\mathcal{K}_{\beta_1\beta_2}(\mathbf{r};\mathbf{r}',\mathbf{k}') = \sum_{\alpha_1\alpha_2} u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})\; u^*_{\alpha_1\alpha_2}(\mathbf{r}',\mathbf{k}')
\tag{3.85}
$$

The new Wigner function can then be regarded as a sort of convolution of the original one with the kernel $\mathcal{K}$ in (3.85). This may recall a well-established procedure used to obtain positive-definite phase-space quantum distributions, the so called "smoothing procedure " [10]. Anyway, that is not true in this case. Indeed, by analyzing the term $\mathcal{K}$ (under the usual hypothesis where $\{\phi\} \equiv \{\chi\}$):

$$
\begin{aligned}
\mathcal{K}_{\beta_1\beta_2}(\mathbf{r};\mathbf{r}',\mathbf{k}') &= \sum_{\alpha_1\alpha_2} u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})\; u^*_{\alpha_1\alpha_2}(\mathbf{r}',\mathbf{k}') \\
&= \sum_{\alpha_1\alpha_2} \int d\mathbf{r}'' \phi_{\alpha_1}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right) \phi^*_{\alpha_2}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right) \phi^*_{\beta_1}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right) \phi_{\beta_2}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right) \cdot \\
&\quad \cdot \int d\mathbf{r}''' \phi^*_{\alpha_1}\left(\mathbf{r}'+\frac{\mathbf{r}'''}{2}\right) \phi_{\alpha_2}\left(\mathbf{r}'-\frac{\mathbf{r}'''}{2}\right) e^{+i\mathbf{k}'\mathbf{r}'''} \\
&= \int d\mathbf{r}'' \delta(\mathbf{r},\mathbf{r}') \phi^*_{\beta_1}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right) \phi_{\beta_2}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right) e^{+i\mathbf{k}'\mathbf{r}''}
\end{aligned}
\tag{3.86}
$$

Thus Eq.(3.84) becomes

$$
\begin{aligned}
f^{WG}_{\beta_1\beta_2}(\mathbf{r}) &= \int d\mathbf{r}' d\mathbf{k}' \delta(\mathbf{r},\mathbf{r}') f^W(\mathbf{r}',\mathbf{k}') \int d\mathbf{r}'' \phi^*_{\beta_1}\left(\mathbf{r}+\frac{\mathbf{r}''}{2}\right) \phi_{\beta_2}\left(\mathbf{r}-\frac{\mathbf{r}''}{2}\right) e^{+i\mathbf{k}'\mathbf{r}''} \\
&= \int d\mathbf{k}' u^*_{\beta_1\beta_2}(\mathbf{r},\mathbf{k}')\; f^W(\mathbf{r},\mathbf{k}')
\end{aligned}
\tag{3.87}
$$

which tells us that the relation between the usual Wigner function and the generalized one involves just the transformation u.

As anticipated, $\mathcal{K}$ is not a conventional convolution. In fact, contrary to usual smoothing procedures -like the Husimi one- here the initial and final phase-space do not coincide, i.e,

$$\mathbf{r}, \mathbf{k} \rightarrow \mathbf{r}, \beta_1, \beta_2$$

To better clarify this point, let us consider the average value of a single-particle physical quantity $\mathcal{A}$. The standard Weyl-Wigner representation leads to

$$\overline{\langle \mathcal{A} \rangle} = Tr[\rho^{sp} \mathcal{A}] = \int d\mathbf{r} d\mathbf{k}\; f^W(\mathbf{r}, \mathbf{k}) \mathcal{A}^W(\mathbf{r}, \mathbf{k}) \tag{3.88}$$

[see Eq.(**??**)]. In the new representation the same average value is given by:

$$\overline{\langle \mathcal{A} \rangle} = Tr[\rho^{sp} \mathcal{A}] = \int d\mathbf{r} \sum_{\beta_1 \beta_2} f^{WG}_{\beta_1 \beta_2}(\mathbf{r}) \mathcal{A}^{WG}_{\beta_1 \beta_2}(\mathbf{r}) = \int d\mathbf{r}\; Tr[f^{WG}(\mathbf{r}) \mathcal{A}^{WG}(\mathbf{r})]_\beta \tag{3.89}$$

with

$$\mathcal{A}^{WG}_{\beta_1 \beta_2}(\mathbf{r}) = \sum_{\alpha_1 \alpha_2} u^{WG}_{\alpha_1 \alpha_2, \beta_1 \beta_2}(\mathbf{r}) \mathcal{A}_{\alpha_1 \alpha_2}$$

As we can see, in the new Weyl-Wigner representation the standard integration over the phase-space $\mathbf{r}, \mathbf{k}$ is replaced by an integration over the real-space coordinate $\mathbf{r}$ plus a trace over the generic quantum number β.

After having analyzed the un-physical results that came out from the usual Weyl-Wigner approach, we are ready to propose a new theoretical model (within the frame of the Generalized Wigner-function approach) able to overcome such problems. In particular, we shall proceed by introducing two different schemes: the first one overcomes the problem of the "distribution symmetry" seen in Fig. 3.3 but still within a non-diagonal injection picture; the second one, in contrast, solves both problems. We shall refer to them respectively as "Model 2" and "Model 3" (by now, we shall refer to the usual Weyl-Wigner approach as "Model 1").

3.2.7 Model 2

Starting from the usual Liouville equation (3.52)

$$\frac{\partial \rho^{sp}_{\alpha_1\alpha_2}}{\partial t} = \sum_{\alpha'_1\alpha'_2} \mathcal{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho^{sp}_{\alpha'_1\alpha'_2}$$

and by applying the inverse of Eq.(3.82), we obtain a Liouville equation in $\beta_1, \beta_2, \mathbf{r}$, i.e.,

$$\frac{d}{dt} f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) = \sum_{\beta'_1\beta'_2} \int d\mathbf{r}' \mathcal{L}^{WG}_{\beta_1\beta_2;\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta'_1\beta'_2}(\mathbf{r}',t) \tag{3.90}$$

This equation is analogous to Eq.(3.55) obtained for "Model 1", but is acting on a different phase-space.

By proceeding in a way similar to what has been done for "Model 1" [see Eq.(3.57)], we can incorporate the desired spatial boundary conditions into the Eq. (3.90):

$$\begin{aligned}\frac{d}{dt} f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) &= \sum_{\beta'_1\beta'_2} \int d\mathbf{r}' \left[\mathcal{L}^{WG}_{\beta_1\beta_2,\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') - |v_{\beta_1}|\, \delta_{\beta_1\beta_2}\delta_{\beta_1\beta'_1}\delta_{\beta_2\beta'_2}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}')\right] f^{WG}_{\beta'_1\beta'_2}(\mathbf{r}',t) \\ &\quad + |v_{\beta_1}|\, \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)} \\ &= \sum_{\beta'_1\beta'_2} \int d\mathbf{r}' \widetilde{\mathcal{L}}^{WG}_{\beta_1\beta_2,\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta'_1\beta'_2}(\mathbf{r}',t) + \widetilde{\mathcal{S}}^{WG}_{\beta_1\beta_2}(\mathbf{r}) \end{aligned} \tag{3.91}$$

with

$$\widetilde{\mathcal{S}}^{WG}_{\beta_1\beta_2}(\mathbf{r}) = |v_{\beta_1}|\, \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)} \tag{3.92}$$

and

$$\widetilde{\mathcal{L}}^{WG}_{\beta_1\beta_2,\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') = \mathcal{L}^{WG}_{\beta_1\beta_2,\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') - |v_{\beta_1}|\, \delta_{\beta_1\beta_2}\delta_{\beta_1\beta'_1}\delta_{\beta_2\beta'_2}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}') \tag{3.93}$$

where v_{β_1} represents the carrier group velocity normal to the boundary surface[10]. An interesting way of writing down Eq.(3.91) is:

$$\frac{d}{dt} f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) = \sum_{\beta'_1\beta'_2} \int d\mathbf{r}' \mathcal{L}^{WG}_{\beta_1\beta_2,\beta'_1\beta'_2}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta'_1\beta'_2}(\mathbf{r}',t)$$

---

[10] Contrary to "Model 1", here the velocity depends on the quantum number β instead of $\mathbf{k}$. However, this does not change the interpretation of the boundary-condition scheme: $r_b = r_{left}$ is related to the injection from left (analogously for r_{right}); in fact, every quantum number β is related to a specific injection (right or left) and this is summarized by the expression $f^{WG}_{b(\beta_1)}$. That means that when β corresponds to injection from left, then $r_b = r_{left}$ (similarly for r_{right}).

$$
\begin{aligned}
& -\sum_{\beta_1'\beta_2'} \int d\mathbf{r}' |v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{\beta_1'\beta_2'}(\mathbf{r}',t) \\
& +|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)} \\
= \ & \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \mathcal{L}^{WG}_{\beta_1\beta_2,\beta_1'\beta_2'}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta_1'\beta_2'}(\mathbf{r}',t) \\
& -|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) \\
& +|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)} \\
= \ & \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \mathcal{L}^{WG}_{\beta_1\beta_2,\beta_1'\beta_2'}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta_1'\beta_2'}(\mathbf{r}',t) \\
& +|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) \left[f^{WG}_{b(\beta_1)} - f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) \right]
\end{aligned}
\tag{3.94}
$$

Such equation has the same role played for "Model 1" by Eq.(3.60). It is possible to show that in steady-state conditions (and in the scattering/dephasing free case) one obtains

$$
f^{WG}_{\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)}) = f^{WG}_{b(\beta_1)}
\tag{3.95}
$$

To demonstrate this result it is sufficient to follow exactly the same steps introduced for "Model 1" [see Eqs. (3.62) and (3.63)].

Going back to the density matrix formalism we get:

$$
\begin{aligned}
\frac{d}{dt}\rho^{sp}_{\alpha_1\alpha_2} = \ & \sum_{\beta_1\beta_2} \int d\mathbf{r}\ u^{*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) \frac{d}{dt} f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) \\
= \ & \sum_{\beta_1\beta_2} \int d\mathbf{r}\ u^{*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) \Bigg\{ \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \Big[\mathcal{L}^{WG}_{\beta_1\beta_2,\beta_1'\beta_2'}(\mathbf{r},\mathbf{r}') + \\
& -|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}') \Big] f^{WG}_{\beta_1'\beta_2'}(\mathbf{r}',t) + \widetilde{\mathcal{S}}^{WG}_{\beta_1\beta_2}(\mathbf{r}) \Bigg\} \\
= \ & \sum_{\beta_1\beta_2} \int d\mathbf{r}\ u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}) \Bigg\{ \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \Big[\sum_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''} u^{WG}_{\alpha_1'\alpha_2',\beta_1\beta_2}(\mathbf{r})\ \mathcal{L}_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''}\ u^{WG,*}_{\alpha_1''\alpha_2'',\beta_1'\beta_2'}(\mathbf{r}') \\
& -|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}') \Big] \sum_{\alpha_1'''\alpha_2'''} \rho^{sp}_{\alpha_1'''\alpha_2'''} u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_2'}(\mathbf{r}') \\
& +|v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)} \Bigg\} \\
= \ & \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \Bigg[\sum_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''} \delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\ \mathcal{L}_{\alpha_1'\alpha_2',\alpha_1''\alpha_2''}\ u^{WG,*}_{\alpha_1''\alpha_2'',\beta_1'\beta_2'}(\mathbf{r}')
\end{aligned}
$$

$$
\begin{aligned}
& -\sum_{\beta_1\beta_2}\int d\mathbf{r}\; u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})|v_{\beta_1}|\;\delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}')\Bigg]\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_2'}(\mathbf{r}') \\
& +\sum_{\beta_1\beta_2}\int d\mathbf{r}\; u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})|v_{\beta_1}|\;\delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b)f^{WG}_{b(\beta_1)} \\
= \;& \sum_{\beta_1'\beta_2'}\int d\mathbf{r}'\Bigg[\sum_{\alpha_1''\alpha_2''}\mathcal{L}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}\; u^{WG,*}_{\alpha_1''\alpha_2'',\beta_1'\beta_2'}(\mathbf{r}') \\
& -\sum_{\beta_1\beta_2}\int d\mathbf{r}\; u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})|v_{\beta_1}|\;\delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}')\Bigg]\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_2'}(\mathbf{r}') \\
& +\sum_{\beta_1\beta_2}u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r}_b)|v_{\beta_1}|\;\delta_{\beta_1\beta_2}\; f^{WG}_{b(\beta_1)} \\
= \;& \sum_{\alpha_1''\alpha_2''}\mathcal{L}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}\;\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}\delta_{\alpha_1''\alpha_1'''}\delta_{\alpha_2''\alpha_2'''} \\
& -\sum_{\beta_1\beta_2,\beta_1'\beta_2'}\int d\mathbf{r}d\mathbf{r}'\; u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_2}(\mathbf{r})|v_{\beta_1}|\;\delta_{\beta_1\beta_2}\delta_{\beta_1\beta_1'}\delta_{\beta_2\beta_2'}\delta(\mathbf{r}-\mathbf{r}_b)\delta(\mathbf{r}-\mathbf{r}') \\
& \cdot\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_2'}(\mathbf{r}')+\sum_{\beta_1}u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_1}(\mathbf{r}_b)|v_{\beta_1}|\; f^{WG}_{b(\beta_1)} \\
= \;& \sum_{\alpha_1''\alpha_2''}\mathcal{L}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}\;\rho^{sp}_{\alpha_1''\alpha_2''}-\sum_{\beta_1'\beta_2'}u^{WG,*}_{\alpha_1\alpha_2,\beta_1'\beta_2'}(\mathbf{r}_b)|v_{\beta_1'}|\delta_{\beta_1'\beta_2'}\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_2'}(\mathbf{r}_b)+\widetilde{\mathcal{S}}_{\alpha_1\alpha_2} \\
= \;& \sum_{\alpha_1''\alpha_2''}\mathcal{L}_{\alpha_1\alpha_2,\alpha_1''\alpha_2''}\;\rho^{sp}_{\alpha_1''\alpha_2''}-\sum_{\alpha_1'''\alpha_2'''}\rho^{sp}_{\alpha_1'''\alpha_2'''}\sum_{\beta_1'}u^{WG,*}_{\alpha_1\alpha_2,\beta_1'\beta_1'}(\mathbf{r}_b)u^{WG}_{\alpha_1'''\alpha_2''',\beta_1'\beta_1'}(\mathbf{r}_b)|v_{\beta_1'}|+\widetilde{\mathcal{S}}_{\alpha_1\alpha_2} \\
= \;& \sum_{\alpha_1'\alpha_2'}\left(\mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}+\Delta\mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\right)\rho^{sp}_{\alpha_1'\alpha_2'}+\widetilde{\mathcal{S}}_{\alpha_1\alpha_2}
\end{aligned}
\tag{3.96}
$$

with

$$
\widetilde{\mathcal{S}}_{\alpha_1\alpha_2}=\sum_{\beta_1}u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)})|v_{\beta_1}|\; f^{WG}_{b(\beta_1)} \tag{3.97}
$$

and

$$
\Delta\mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}=-\sum_{\beta_1}|v_{\beta_1}|\; u^{WG,*}_{\alpha_1\alpha_2,\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)})\; u^{WG}_{\alpha_1'\alpha_2',\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)}) \tag{3.98}
$$

Here, the source term $\widetilde{\mathcal{S}}_{\alpha_1\alpha_2}$ has not a diagonal nature so that the model here described, "Model 2", is not adequate to describe a thermal/diagonal injection. However, within the present model the "symmetry problem" previously encountered (see Fig. 3.3) has been removed; the new microscopic result is found to be in good agreement with that of the phenomenological model, as reported in Fig. 3.4.

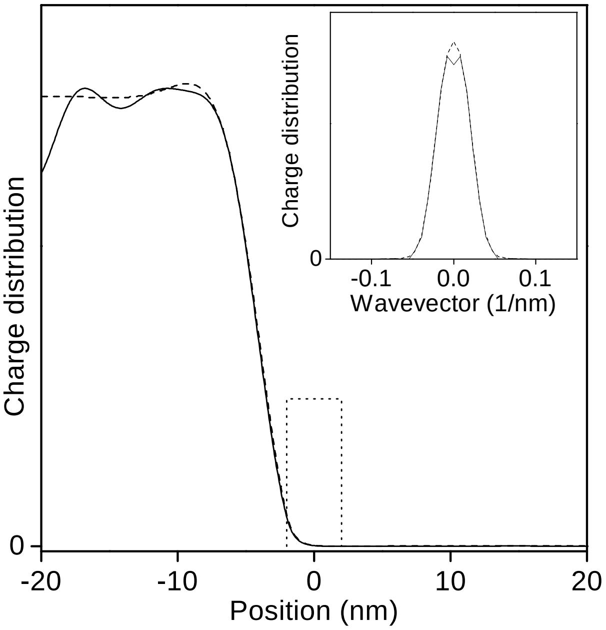

Figure 3.4: Comparison between the real-space charge distribution obtained from the phenomenological injection model in Eq.(3.76) [$n(\mathbf{r}) = \sum_\alpha f_\alpha |\phi_\alpha(\mathbf{r})|^2$ - dashed curve] and the microscopic model in Eq.(3.96)/Eq.(3.103) [$n(\mathbf{r}) = \sum_{\alpha_1\alpha_2} \rho^{sp}_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r})\phi^*_{\alpha_2}(\mathbf{r})$ - solid curve] for a GaAs-based single barrier structure (height $V_0 = 0.5eV$ and width $a = 4nm$) equidistant from the electrical contacts. In this room-temperature simulation, due to a misalignment $\Delta\mu = 0.2eV$ of the left and right chemical potential, carriers are primarily injected from left. The corresponding charge distribution in momentum space is also reported in the inset.

To solve also the problem of non-diagonality of $\widetilde{\mathcal{S}}_{\alpha_1\alpha_2}$, let us introduce a new scheme, that we shall call "Model 3".

3.2.8 Model 3

This second approach to open systems starts from the same initial equation (3.91) used for "Model 2", i.e.,

$$\frac{d}{dt} f^{WG}_{\beta_1\beta_2}(\mathbf{r},t) = \sum_{\beta_1'\beta_2'} \int d\mathbf{r}' \widetilde{\mathcal{L}}^{WG}_{\beta_1\beta_2,\beta_1'\beta_2'}(\mathbf{r},\mathbf{r}') f^{WG}_{\beta_1'\beta_2'}(\mathbf{r}',t) + \widetilde{\mathcal{S}}^{WG}_{\beta_1\beta_2}(\mathbf{r})$$

with

$$\widetilde{\mathcal{S}}^{WG}_{\beta_1\beta_2}(\mathbf{r}) = |v_{\beta_1}|\ \delta_{\beta_1\beta_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\beta_1)}$$

Contrary to "Model 2", here we employ the relationship

$$\rho^{sp}_{\alpha_1\alpha_2} = \int d\mathbf{r} f^{WG}_{\alpha_1\alpha_2}(\mathbf{r}) \tag{3.99}$$

The latter can be easily demonstrated as follows:

$$\begin{aligned} \int d\mathbf{r} f^{WG}_{\alpha_1\alpha_2}(\mathbf{r}) &= \int d\mathbf{r} \sum_{\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} u^{WG}_{\beta_1\beta_2,\alpha_1\alpha_2}(\mathbf{r}) \\ &= \sum_{\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} \int d\mathbf{r} u^{WG}_{\beta_1\beta_2,\alpha_1\alpha_2}(\mathbf{r}) \\ &= \sum_{\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} \langle \alpha_1|\beta_1\rangle\langle\beta_2|\alpha_2\rangle \\ &= \rho^{sp}_{\alpha_1\alpha_2} \end{aligned}$$

where we have assumed again $\{\phi\} \equiv \{\chi\}$.

Thus, by means of Eq.(3.99), let us develop the equation of motion for the density matrix:

$$\begin{aligned} \frac{d}{dt}\rho^{sp}_{\alpha_1\alpha_2} &= \int d\mathbf{r} \frac{d}{dt} f^{WG}_{\alpha_1\alpha_2}(\mathbf{r}) \\ &= \int d\mathbf{r} \Big\{ \sum_{\alpha_1'\alpha_2'} \int d\mathbf{r}' \Big[\mathcal{L}^{WG}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}(\mathbf{r},\mathbf{r}') - |v_{\alpha_1}|\ \delta_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b)\Big] f^{WG}_{\alpha_1'\alpha_2'}(\mathbf{r}') + \\ &\quad |v_{\alpha_1}|\ \delta_{\alpha_1\alpha_2}\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{b(\alpha_1)} \Big\} \end{aligned}$$

$$
\begin{aligned}
&= \int d\mathbf{r}\Big\{ \sum_{\alpha_1'\alpha_2'} \int d\mathbf{r}' \Big[\sum_{\beta_1\beta_2,\beta_1'\beta_2'} u^{WG}_{\beta_1\beta_2,\alpha_1\alpha_2}(\mathbf{r}) \mathcal{L}_{\beta_1\beta_2,\beta_1'\beta_2'} u^{WG,*}_{\beta_1'\beta_2',\alpha_1'\alpha_2'}(\mathbf{r}') f^{WG}_{\alpha_1'\alpha_2'}(\mathbf{r}') - \\
&\quad |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{\alpha_1'\alpha_2'}(\mathbf{r}')\Big]\Big\} + |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2} f^{WG}_{b(\alpha_1)} \\
&= \sum_{\alpha_1'\alpha_2',\beta_1'\beta_2'} \int d\mathbf{r}' L_{\alpha_1\alpha_2,\beta_1'\beta_2'} u^{WG,*}_{\beta_1'\beta_2',\alpha_1'\alpha_2'}(\mathbf{r}') f^{WG}_{\alpha_1'\alpha_2'}(\mathbf{r}') - \\
&\quad \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha_1'\alpha_2'} |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b) f^{WG}_{\alpha_1'\alpha_2'}(\mathbf{r}') + |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2} f^{WG}_{b(\alpha_1)} \\
&= \sum_{\alpha_1'\alpha_2',\beta_1'\beta_2'} \int d\mathbf{r}' L_{\alpha_1\alpha_2,\beta_1'\beta_2'} u^{WG,*}_{\beta_1'\beta_2',\alpha_1'\alpha_2'}(\mathbf{r}') \sum_{\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} u^{WG}_{\beta_1\beta_2,\alpha_1'\alpha_2'}(\mathbf{r}') - \\
&\quad \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha_1'\alpha_2'} |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_b) \sum_{\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} u^{WG}_{\beta_1\beta_2,\alpha_1'\alpha_2'}(\mathbf{r}') + |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2} f^{WG}_{b(\alpha_1)} \\
&= \sum_{\beta_1\beta_2} \mathcal{L}_{\alpha_1\alpha_2,\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} - \sum_{\beta_1\beta_2,\alpha_1'\alpha_2'} |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'} u^{WG}_{\beta_1\beta_2,\alpha_1'\alpha_2'}(\mathbf{r}_{b(\alpha_1)}) \rho^{sp}_{\beta_1\beta_2} + |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2} f^{WG}_{b(\alpha_1)} \\
&= \sum_{\beta_1\beta_2} \Big[\mathcal{L}_{\alpha_1\alpha_2,\beta_1\beta_2} - |v_{\alpha_1}|\, u^{WG}_{\beta_1\beta_2,\alpha_1'\alpha_2'}(\mathbf{r}_{b(\alpha_1)})\, \delta_{\alpha_1\alpha_2}\Big] \rho^{sp}_{\beta_1\beta_2} + |v_{\alpha_1}|\, \delta_{\alpha_1\alpha_2} f^{WG}_{b(\alpha_1)} \\
&= \sum_{\beta_1\beta_2} \Big[\mathcal{L}_{\alpha_1\alpha_2,\beta_1\beta_2} + \Delta\mathcal{L}_{\alpha_1\alpha_2,\beta_1\beta_2}\Big] \rho^{sp}_{\beta_1\beta_2} + \widetilde{\mathcal{S}}_{\alpha_1\alpha_2}
\end{aligned}
\tag{3.100}
$$

As desired, within this new scheme the source term $\widetilde{\mathcal{S}}$ is diagonal.

If we now analyze the non-diagonal case of Eq.(3.100), i.e., $\alpha_1 \neq \alpha_2$ we have:

$$
\frac{d}{dt}\rho^{sp}_{\alpha_1\alpha_2} = \sum_{\beta_1\beta_2} \mathcal{L}_{\alpha_1\alpha_2,\beta_1\beta_2} \rho^{sp}_{\beta_1\beta_2} \tag{3.101}
$$

i.e., if at time $t = 0$ we have $\rho^{sp}_{\alpha_1\alpha_2} = 0$, then it remains equal to zero forever; namely, within "Model 3", the density matrix ρ^{sp} is diagonal.

Our simulated experiments have shown that this last model leads exactly to the same results obtained for "Model2", reported in Fig. 3.4. This is not particularly surprising if one considers that both models start from the same equation (3.91). Generally speaking, we can conclude that we deal with a sort of gauge freedom, which tells us that the source term in our effective density-matrix equation must not necessarily be diagonal.

Similarly to Model 2, it is possible to show that Eq.(3.95) works also for Model 3, namely

$$
f^{WG}_{\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)}) = f^{WG}_{b(\beta_1)}
$$

But, in the new model, such a relation has a very important conceptual consequence, i.e., it tells us that the distribution function in state α is the result of an "incoherent superposition" from all the injection channels. In fact:

$$f^{WG}_{b(\beta_1)} = f^{WG}_{\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)}) = \sum_{\alpha_1\alpha_2} u^{WG}_{\alpha_1\alpha_2,\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)})\rho^{sp}_{\alpha_1\alpha_2}$$

but, as shown, ρ^{sp} is diagonal so that the previous equation becomes

$$f^{WG}_{b(\beta_1)} = \sum_{\alpha_1} u^{WG}_{\alpha_1\alpha_1,\beta_1\beta_1}(\mathbf{r}_{b(\beta_1)})\rho^{sp}_{\alpha_1\alpha_1}$$

which written in compact form becomes

$$f^{WG}_{b(\beta)} = \sum_{\alpha} \tau_{\alpha\beta} f_\alpha \qquad (3.102)$$

Equation (3.102) is semiclassical in nature, i.e., it involves diagonal density-matrix terms only. However, contrary to the phenomenological injection model in (3.76), here the distribution function f_α comes from an "incoherent superposition" of all the injection channels, i.e.,

$$f_\alpha = \sum_{\beta} \tau^{-1}_{\alpha\beta}\, f^{WG}_{b(\beta)} \qquad (3.103)$$

If the term $\tau_{\alpha\beta} = \delta_{\alpha\beta}$ the phenomenological injection model is recovered. Figure 3.4 shows again results for the single-barrier potential profile. Here, the simulation based on the phenomenological injection model in Eq.(3.76) (dashed curves) is compared to that of the new microscopic model in (3.103) (solid curves). As we can see, the highly non physical behaviours of Fig. 3.3 (solid curve) has been completely removed. Indeed, the momentum distribution in the inset is always positive-definite and the two models exhibit a very similar behaviour. We can see relatively small deviations close to the device spatial boundaries, which can be ascribed to the interlevel injection coupling $\tau_{\alpha\beta}$ (inside the Model 2, τ would have a more complicated form but with similar meaning), not present in the phenomenological injection model. This is clearly a fingerprint of our real-space description, where the point-like carrier injection is located at the device spatial boundaries. However, when the device active region is relatively far from the contacts these deviations can be safely neglected, and the phenomenological model provide reliable results.

Chapter 4

Summary and conclusions

A deep analysis of the various approximations entering in charge transport semiclassical theory reveals that in physical systems it is more and more fundamental to adopt a quantum nature approach to study transport phenomena. Although the basis ideas of quantum transport theory are already known since years, so far a clear and definitive approach able to solve the problem of quantum open system was not yet a reality. Indeed, in this work we have proposed a rigorous description of quantum-transport phenomena in systems with open boundaries that, we believe, is able to solve the quantum-open-system problem.

Our analysis has shown that the conventional Wigner-function formalism —when applied to charge transport in nanostructured open systems— leads to unphysical results; This basic limitation has been removed by introducing a generalization of the standard Wigner-function formalism, able to properly describe the incoherent nature of carrier injection. The proposed theoretical approach allowed us to obtain results in good agreement with that of the phenomenological model, thus guaranteeing the validity and relevance of the proposed theoretical framework.

A strongly-related aspect faced in our work is the problem of a coherent vs. incoherent source term. In fact, from our analysis it follows that source terms —describing incoherent carrier injection into the device active region— should exhibit thermal, i.e., incoherent, properties, inasmuch as they represent the environment, namely the external world in thermodynamic contact with the carrier subsystem under investigation. Anyway, we have clarified that the classification in terms of “incoherent” (diagonal) and “coherent” (non-diagonal) is somewhat artificial, since it is basis-dependent. It follows that via a proper basis transformation we may go from a diagonal to a non-diagonal source term.

By concluding, we believe that our approach could represent a relevant step forward in properly defining a theoretical model —and a corresponding simulation strategy— able to treat any generic quantum transport problem in open optoelectronic devices.

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