

# Decoherence and Quantum Transport in Nanodevices

I. Knezevic

*Department of Electrical and Computer Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA*

In nanoscale, quasiballistic devices, the process of relaxation towards a steady state cannot be attributed to efficient carrier scattering, and can therefore no longer be described by the Boltzmann equation. Instead, a nanodevice's active region is an open quantum-mechanical system, and its relaxation is determined by the process of decoherence due to the injection of carriers from the leads. In this paper, a formalism that captures decoherence as the dominant mechanism of relaxation in nanodevices is introduced. By working within a projection-operator technique, commonly used in the open systems theory, a Markovian approximation for an abstract open system's evolution is derived through coarse-graining of the exact short-time dynamics. This Markovian approximation faithfully represents the long-time stages of evolution, and correctly identifies the nonequilibrium steady state directly from first principles. Relaxation in a ballistic resonant-tunneling diode is described in detail within the presented formalism, and the resulting steady-state I–V curve displays the prominent resonant features.

**Keywords:** Decoherence, Quantum Transport, Open System, Contacts, Nanostructure, Nanodevice, Non-Markovian Dynamics, Markovian Dynamics, Projection Operator Technique, Relaxation, Steady State, Resonant Tunneling Diode.

## 1. INTRODUCTION

The small and fast semiconductor device of the present is an exciting quantum-mechanical system: it features virtually collision-free transport, very few carriers in the active region, significant inter-carrier correlations, and the switching speed determined by the process of decoherence due to interaction with the leads that supply both charge and information. Since the device dimensions are smaller than the carrier mean-free path even at room temperature, solving the semiclassical Boltzmann transport equation (BTE)<sup>1,2</sup> to characterize transport ceases to yield credible results. The main reason is that its premise—frequent scattering governing relaxation—no longer holds, so the very validity of the BTE as the kinetic equation is questioned. Significant efforts have been aimed at establishing a full quantum transport description of ultrasmall devices, the most widespread approaches being the density matrix approach,<sup>3–8</sup> Wigner functions,<sup>9–16</sup> and nonequilibrium Green's functions.<sup>17–23</sup> Recent work by Fischetti<sup>24,25</sup> shows that an adequate quantum description of small devices may be obtained by replacing the Boltzmann equation with the Pauli master equation for the diagonal elements of the density matrix, with the complexity of the approach similar to Schrödinger-Poisson-Monte Carlo solvers. However, in the presence of contacts, the off-diagonal density matrix elements are appreciable,<sup>26,27</sup> and neglecting them may violate current continuity.

The importance of treating a nanoscale device as an open quantum system interacting with the contacts was first thoroughly discussed by Pötz<sup>28</sup> and Frensley,<sup>26</sup> and more recently others.<sup>29–34</sup> In the low-field, steady state regime, the variant of nonequilibrium Green's functions formalism introduced by Datta and coworkers<sup>18,20,21</sup> accounts for the open boundaries through a special injection self-energy term, where the electrons are injected from each contact with the contact's equilibrium distribution. However, there is no kinetic theory showing that this is indeed the steady state that the system relaxes to upon the application of bias, nor how the results would look in the high field regime or during the transients. It is now well accepted that the treatment of contacts<sup>31,34,35</sup> is crucial for describing the relaxation in the absence of frequent scattering. However, a general description of the contact-induced decoherence (nonunitary dynamics) in nanoscale devices is lacking.

In this paper, I introduce the basics of a formalism that captures the decoherence in a nanodevice's active region due to its interaction and particle exchange with the contacts (reservoirs) as the essential mechanism through which a steady state is achieved. In Section 2, I introduce the core elements of the partial-trace-free (PTF) technique<sup>36</sup> for treatment of the dynamics of an abstract open system. The PTF approach and the resulting equations with memory dressing,<sup>37</sup> overviewed here, are a special variant of a wide class of projection operator

techniques,<sup>38,39</sup> that are a popular way to treat open systems (usually small ones) in quantum information theory. In Section 2.2, we will focus on obtaining the long-time limit of the evolution from first principles, and show that it can be done via coarse-graining of the exact non-Markovian evolution over very short times. The main point of the paper is that the steady state of an open system, such as the active region of a nanodevice, can be obtained in completely general terms and without tracking all the details of the evolution, just from the microscopic interaction Hamiltonians and the state of its environment, as demonstrated at the end of Section 2.2. Proper relaxation has been demonstrated on two simple examples in Section 2.3, and, in Section 3, the formalism is applied to the case of a ballistic resonant-tunneling diode (RTD). Steady-state distributions for the forward and backward propagating states are calculated, and used to compute the steady-state I-V curve, that properly displays all the resonant features. The paper ends with concluding remarks in Section 4.

## 2. NANODEVICE AS AN OPEN QUANTUM SYSTEM—THE FORMALISM

In this section, I will introduce the basics of an open-system formalism used to treat the dynamics of the nanodevices. We will start by deriving a non-Markovian dynamical law for the evolution of an abstract open system's density matrix. "Non-Markovian" means that the memory effects are important,<sup>40</sup> i.e., that the environment E retains memory on the timescale relevant for the system evolution. In contrast, Markovian<sup>40–43</sup> (memoryless) evolution corresponds to the environment losing memory on timescales much shorter than the system characteristic times. Physically, environment typically loses memory because of its large number of degrees of freedom, so that all the information obtained from the small system gets dissipated over some correlation-decay time of the environment. For instance, systems weakly coupled to large, thermal environments will behave in a Markovian fashion on timescales larger than the thermal time  $\hbar/k_B T$ , which is a typical time for the destruction of correlations in a thermal environment. Markovian evolution is characterized by an exponential decay of certain components of the density matrix. A number of famous master equations for the evolution of different open systems are Markovian, such as the Pauli master equation,<sup>44</sup> Caldeira-Leggett equation,<sup>45</sup> Redfield equation,<sup>46</sup> and optical Bloch equations.<sup>47</sup>

### 2.1. Decomposition of the Liouville Space. Equations with Memory Dressing

Let us consider an open system S, coupled with the environment E, so that the composite SE is closed. These

systems are assumed to have finite-dimensional Hilbert spaces, of dimensions  $d_S$ ,  $d_E$ , and  $d_S d_E$ , respectively. Consequently, their Liouville spaces—the spaces of operators acting on the above Hilbert spaces—are of dimensions  $d_S^2$ ,  $d_E^2$ , and  $d_S^2 d_E^2$ , respectively. The total SE Hamiltonian  $\mathcal{H}$  is generally a sum of a system part  $1_E \otimes \mathcal{H}_S$ , an environment part  $\mathcal{H}_E \otimes 1_S$ , and an interaction part  $\mathcal{H}_{int}$ . The total Hamiltonian  $\mathcal{H}$  (acting on the SE Hilbert space) induces the total SE Liouvillian  $\mathcal{L}$  (acting on the SE Liouville space) through the commutator, which governs the evolution of the SE density matrix  $\rho$  according to the Liouville equation

$$\frac{d\rho}{dt} = -i[\mathcal{H}, \rho] = -i\mathcal{L}\rho \quad (1)$$

Dynamics of the open system S is described by its reduced density matrix  $\rho_S$ , obtained from  $\rho$  by tracing out the environment states

$$\rho_S = \text{Tr}_E \rho \quad (2)$$

In general, the dynamics of  $\rho_S$  is not unitary. A common approach to calculating the evolution of  $\rho_S$  is by using projection operators<sup>38,39,47</sup> that act on the SE Liouville space. Typically, an environmental density matrix  $\rho_E$  is chosen to induce a projection operator  $P$  by  $P\rho = \rho_E \otimes \text{Tr}_E \rho$ , where  $\mu$  is any vector from the SE Liouville space. Coupled equations of motion for  $P\rho$  and  $(1-P)\rho$  are then solved, often in the weak-coupling limit, and the reduced dynamics is obtained from  $\rho_S = \text{Tr}_E \rho = \text{Tr}_E (P\rho)$ .

Most often, the projection operator utilized is induced by the initial environmental density matrix  $\rho_E(0)$ .<sup>47</sup> The reason is that, in the most common approximation of initially decoupled S and E, described by  $\rho(0) = \rho_E(0) \otimes \rho_S(0)$ , the projection operator induced by  $\rho_E(0)$  will eliminate a certain memory term occurring in the evolution of  $\rho_S$ . However, the result for the final dynamics must not depend on the projection operator used, as projection operators are, after all, only auxiliary quantities. In this paper, we will follow the work on the partial-trace-free approach of Ref. [36], that uses the projection operator  $\bar{P}$  induced by the uniform environment density matrix  $\bar{\rho}_E = d_E^{-1} \text{diag}(1 \dots 1)$ .  $\bar{P}$  has a unique property: it is the only projection operator that has an orthonormal eigenbasis in which it is represented by a diagonal form. Its unit eigenspace, of dimension  $d_S^2$ , is a mirror-image of the Liouville space of the open system S. *Projecting onto the unit eigenspace of  $\bar{P}$  is equivalent to taking the partial trace with respect to environmental states*,<sup>36</sup> because for any element of the SE Liouville space it holds

$$(\bar{P}\mu)^{\bar{\alpha}\bar{\beta}} = d_E^{-1/2} (\text{Tr}_E \mu)^{\alpha\beta} \quad (3)$$

Here, the unit-eigenspace of  $\bar{P}$  is spanned by a basis  $|\bar{\alpha}\bar{\beta}\rangle$ , while the Liouville space of S is spanned by  $|\alpha\beta\rangle$ , where the two bases are isomorphic through the following simple relationship

$$|\bar{\alpha}\bar{\beta}\rangle = d_E^{-1/2} \sum_{j=1}^{d_E} |j\alpha, j\beta\rangle \quad (4)$$

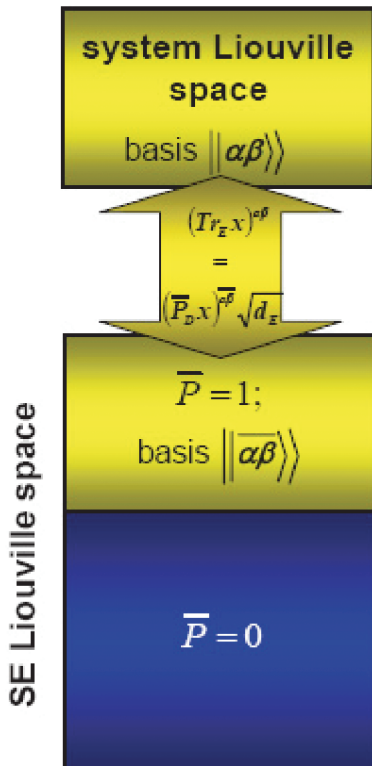
$|i\alpha, j\beta\rangle$  is a basis in the SE Liouville space, induced by the bases  $|ij\rangle$  and  $|\alpha\beta\rangle$  in the environment and system Liouville spaces, respectively.

Decomposition of the SE Liouville space into the two eigenspaces of  $\bar{P}$  (depicted in Fig. 1) is the essence of the PTF approach: every vector  $\mu$  from the SE Liouville space can be written as a column  $\mu = [\mu_1, \mu_2]^T$ , where  $\mu_1$  belongs to the unit eigenspace of  $\bar{P}$  and represents (up to a multiplicative constant  $\sqrt{d_E}$ ) the system's reduced component of  $\mu$ , i.e.,  $\mu_S \equiv \text{Tr}_E \mu = \sqrt{d_E} \mu_1$ . The other component,  $\mu_2$ , belongs to subspace 2 (the zero-eigenspace of  $\bar{P}$ ), where the correlations between S and E reside. It is important to note that the elements of subspace 2 (blue subspace in Fig. 1) have zero trace over environmental states.

In a similar fashion, an operator  $A$  acting on the SE Liouville space has a block-form with submatrices  $A_{pq}$ ,  $p, q = 1, 2$ , where  $A_{11}$  would be the system's reduced component of this operator. For instance, the block form of the SE Liouvillian  $L$  is given by

$$L = \begin{bmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} \\ \mathcal{L}_{21} & \mathcal{L}_{22} \end{bmatrix}$$

where  $\mathcal{L}_{11}$  is commutator-generated, and corresponds to an effective system Hamiltonian  $\mathcal{H}_S + \text{Tr}_E(\mathcal{H}_{\text{int}})/d_E$ .



**Fig. 1.** Decomposition of the total SE Liouville space into the eigenspaces of the projection operator  $\bar{P}$ , induced by the uniform density matrix  $\bar{\rho}_E$ . The unit eigenspace is equivalent to the system Liouville space, where the equivalence is given by the isomorphism (3). Working within the eigenspaces of  $\bar{P}$  removes the need for performing the partial trace over the environmental states.

Off-diagonal, non-square Liouvillian submatrices,  $\mathcal{L}_{12}$  and  $\mathcal{L}_{21} = \mathcal{L}_{12}^\dagger$ , represent the S–E interaction as seen in the composite Liouville space—when  $\mathcal{H}_{\text{int}}$  vanishes, so do  $\mathcal{L}_{12}$  and  $\mathcal{L}_{21}$ .  $\mathcal{L}_{22}$  can be perceived as governing the evolution of entangled SE states, and tends to a form fixed by  $\mathcal{H}_S$  and  $\mathcal{H}_E$  when the interaction is turned off.

Using the notation introduced above, the evolution of the reduced density matrix  $\rho_S$  can be represented by

$$\rho_S(t) = \mathcal{U}_{11}(t, 0)\rho_S(0) + \sqrt{d_E}\mathcal{U}_{12}(t, 0)\rho_2(0) \quad (5)$$

where  $\mathcal{U}_{11}$  and  $\mathcal{U}_{12}$  are the submatrices of the SE evolution operator  $\mathcal{U}$ , given by

$$\begin{aligned} \mathcal{U}(t, 0) &= \text{T}^c \exp\left(-i \int_0^t \begin{bmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} \\ \mathcal{L}_{21} & \mathcal{L}_{22} \end{bmatrix} dt\right) \\ &= \begin{bmatrix} \mathcal{U}_{11}(t, 0) & \mathcal{U}_{12}(t, 0) \\ \mathcal{U}_{21}(t, 0) & \mathcal{U}_{22}(t, 0) \end{bmatrix} \end{aligned}$$

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In Ref. [37], equations of motion for  $\mathcal{U}_{11}$  and  $\mathcal{U}_{12}$  were derived as

$$\frac{d\mathcal{U}_{11}}{dt} = -i(\mathcal{L}_{11} - \mathcal{L}_{12}\mathcal{R})\mathcal{U}_{11} \quad (6a)$$

$$\frac{d\mathcal{U}_{12}}{dt} = -i(\mathcal{L}_{11} - \mathcal{L}_{12}\mathcal{R})\mathcal{U}_{12} - i\mathcal{L}_{12}\mathcal{V} \quad (6b)$$

accompanied by the initial conditions  $\mathcal{U}_{11}(0, 0) = 1$  and  $\mathcal{U}_{12}(0, 0) = 0$ . Quantity  $\mathcal{R}$  is the so-called *memory dressing*, as it appears to “dress” the real physical interaction  $\mathcal{L}_{12}$  and yield an effective (generally complex) interaction term,  $-\mathcal{L}_{12}\mathcal{R}$ , that accompanies the hermitian term  $\mathcal{L}_{11}$ , responsible for unitary evolution. Memory dressing describes the cumulative effect of the S–E interaction, as witnessed by a quadratic feedback term in its self-contained matrix Riccati<sup>48, 49</sup> equation of motion (below). The other new quantity occurring in (6),  $\mathcal{V}(t, 0)$ , can be perceived as the evolution operator for the states from subspace 2, and is important for the description of the influx of information from E to S.  $\mathcal{R}$  and  $\mathcal{V}$  obey

$$\frac{d\mathcal{R}}{dt} = -i\mathcal{L}_{22}\mathcal{R} - i\mathcal{R}\mathcal{L}_{12}\mathcal{R} + i\mathcal{R}\mathcal{L}_{11} + i\mathcal{L}_{21} \quad (7a)$$

$$\frac{d\mathcal{V}}{dt} = -i(\mathcal{L}_{22} + \mathcal{R}\mathcal{L}_{12})\mathcal{V} \quad (7b)$$

accompanied by  $\mathcal{R}(0) = 0$  and  $\mathcal{V}(0, 0) = 1$ .

Equations (6) and (7) are *exact*:<sup>37</sup> they are an alternative form of the SE Liouville Equation (1). The resulting exact evolution of the reduced density matrix can be expressed through the following differential equation of motion

$$\begin{aligned} \frac{d\rho_S(t)}{dt} &= -i[\mathcal{L}_{11} - \mathcal{L}_{12}\mathcal{R}(t)]\rho_S(t) \\ &\quad - i\mathcal{L}_{12}\sqrt{d_E}\mathcal{V}(t, 0)\rho_2(0) \end{aligned} \quad (8)$$

which is a partial-trace-free form of  $d\rho_S/dt = \text{Tr}_E(-iL\rho)$ .

If we restrict our attention to the evolution starting from an initially uncorrelated state of the form

$$\rho(0) = \rho_E(0) \otimes \rho_S(0) \quad (9)$$

it is possible to completely reduce the problem to subspace 1. Namely, it is possible to write

$$\rho_2(0) = \mathcal{M}\rho_1(0) = d_E^{-1/2} \mathcal{M}\rho_S(0) \quad (10)$$

where the mapping  $\mathcal{M}$  is completely determined by the components of  $\rho_E(0)$ , the initial environment density matrix.<sup>50</sup> Equation (10) embodies the argument made by Lindblad<sup>51</sup> that a subdynamics exists only for an uncorrelated initial state, because, as a consequence of (5) and (10), it is possible to write

$$\rho_S(t) = [\mathcal{U}_{11}(t, 0) + \mathcal{U}_{12}(t, 0)\mathcal{M}]\rho_S(0) \quad (11)$$

so the evolution is completely described on the Liouville space of the open system. Consequently, when (10) is substituted into (8), we obtain

$$\frac{d\rho_S(t)}{dt} = -i[\mathcal{L}_{11} - \mathcal{L}_{12}\mathcal{R}(t)]\rho_S(t) - i\mathcal{L}_{12}\mathcal{V}(t)\mathcal{M}\rho_S(0) \quad (12)$$

## 2.2. Long-Time Markovian from the Short-Time Non-Markovian Decoherence

Equation (12) is in principle impossible to solve exactly, and typically expansion up to the second or fourth order in terms of the interaction is undertaken. For a comprehensive overview of the time-convolutionless projection operator technique, see Chapter 4 of Ref. [47]. Unfortunately, the resulting equations can violate positivity of the density matrix, which can potentially lead to unphysical results. Furthermore, in solid state physics one cannot always justify the weak-coupling approximation, such as in the case of carrier-carrier interaction. However, there are other simplifications we can make to address decoherence in nanoscale devices:

- (1) First, the details of transient are often not important *per se*, especially in devices used for digital applications. A good estimate of the relaxation time is usually enough.
- (2) Along the same lines, a good approximation for the non-equilibrium steady state is perhaps the most important information that needs to come from any simulator of a device used for digital applications.
- (3) The full density matrix of the whole electronic system is not needed. Usually, the few lowest order Green's functions are enough to characterize current transport.

Therefore, we need to find a good, numerically tractable way to obtain the nonequilibrium steady state many-body density matrix in a general form, so that we would be in principle able to extract the single-particle Green's functions we typically use for transport calculations.

In the rigorous theory of open systems, it is well-known from the seminal work of Davies<sup>43</sup> that the exact non-Markovian evolution, described by (12), can be approximated via a Markovian map (local in time) on appropriately rescaled timescales (i.e., in the so-called van Hove limit)<sup>41,42</sup> when one is dealing with a system weakly coupled to a large environment. Here, we want to pose the problem somewhat differently: Suppose that, on the timescales of interest in experiment, you are confident that you will observe Markovian-type evolution [exponential decay towards a steady state], and that you have little interest in the short-time, non-Markovian effects. *How do you obtain this Markovian evolution from the microscopic model Hamiltonians and the initial state of the environment?* There are several ways to obtain Markovian equations from non-Markovian ones, depending on the premises used. Among them is the approach of *coarse graining* the non-Markovian evolution with respect to the time over which the environment retains memory. Coarse graining, although shown to retain the complete positivity of the map (12),<sup>52</sup> always carries a degree of arbitrariness as to how long the coarse graining time is actually supposed to be.<sup>43</sup>

Here, we will postulate the following: *For a non-Markovian open system coupled to a large bath, which exhibits Markovian evolution in the long-time limit, there exists a coarse-graining time  $\tau$  that is shorter than any timescale characteristic for either the system or the environment, such that the Markovian evolution obtained by coarse graining over  $\tau$  is the same as the long-time limit of the exact non-Markovian evolution.*

The ultrashort  $\tau$  enables us to utilize the *short-time expansion* of the exact non-Markovian evolution, which we can deduce relatively straightforwardly from the initial preparation of S and E and the Hamiltonians, to obtain the eventual long-time steady state! A formal proof of the postulate for boson baths in the limit of weak coupling will be published elsewhere.<sup>50</sup> It is very important to note that  $\tau$  is a *mathematical coarse-graining time*, it is *not* the physical time corresponding to a decay of environmental correlations (which is of order  $\hbar/k_B T$  for thermal bosonic baths, for example). Indeed, in Section 2.3, on an exactly solvable model we will indeed show that  $\tau$  sets by far the shortest timescale in the system.

So we will first rewrite the exact non-Markovian evolution compactly as

$$\rho_S(t) = T^c \exp \left[ -i \int_0^t \mathcal{L}_{\text{eff}}(\tau) d\tau - \Gamma(t) \right] \rho_S(0) \quad (13)$$

where  $\mathcal{L}_{\text{eff}}(t)$  is a still undetermined effective Liouvillian, and  $\Gamma(t)$  is the decoherence exponent. This form holds without the loss of generality;<sup>40</sup> for instance, it definitely holds in the Markov approximation, where the so-called *semigroup generator*  $-i\mathcal{L}_{\text{eff}} - d\Gamma/dt = \text{const.}$ , of the well-known Lindblad form,<sup>53,54</sup> generates a so-called

completely positive evolution. Complete positivity of a dynamical map means that the unit trace and positivity of the density matrix are preserved at all times, but also that the evolution is robust enough to support tensor products—for example, two noninteracting systems evolving according to completely positive maps can together be described by a tensor product of those maps, itself a completely positive map.

We will perform the short-time Taylor expansion of the exact Equation (12) up to the second order in time

$$\left(\frac{d\rho_S}{dt}\right)_0 = \left[-i\mathcal{L}_{\text{eff}}(0) - \left(\frac{d\Gamma}{dt}\right)_0\right]\rho_S(0) \quad (14a)$$

$$\begin{aligned} \left(\frac{d^2\rho_S}{dt^2}\right)_0 &= \left[-i\left(\frac{d\mathcal{L}_{\text{eff}}}{dt}\right)_0 - \left(\frac{d^2\Gamma}{dt^2}\right)_0\right]\rho_S(0) \\ &+ \left[-i\mathcal{L}_{\text{eff}}(0) - \left(\frac{d\Gamma}{dt}\right)_0\right]^2\rho_S(0) \end{aligned} \quad (14b)$$

which will then help us identify the short-time incarnations of the effective Liouvillian and the decoherence exponent  $\Gamma$ , that we will later be able to use for coarse graining. Without going into the details, we obtain

$$\mathcal{L}_{\text{eff}}(0) = \mathcal{L}_{11} + \mathcal{L}_{12}\mathcal{M} = [\mathcal{H}_S + \langle\mathcal{H}_{\text{int}}\rangle, \dots], \quad (15a)$$

$$\left(\frac{d\mathcal{L}_{\text{eff}}}{dt}\right)_0 = 0$$

$$\left(\frac{d\Gamma}{dt}\right)_0 = 0, \quad \left(\frac{d^2\Gamma}{dt^2}\right)_0 = 2\Lambda \quad (15b)$$

where  $\langle\cdots\rangle = \text{Tr}_E\langle\rho_E(0)\cdots\rangle$  denotes the partial environmental average with respect to the initial environmental state  $\rho_E(0)$ , and the operator  $\Lambda$  is defined as

$$\begin{aligned} \Lambda_{\alpha\beta}^{\alpha'\beta'} &= \frac{1}{2} \sum_k \rho_E^k \left\{ (\mathcal{H}_{\text{int}}^2)_{k\alpha}^{k\alpha'} \delta_{\beta}^{\beta'} - 2 \sum_{k'} (\mathcal{H}_{\text{int}})_{k\alpha}^{k'\alpha'} (\mathcal{H}_{\text{int}})_{k'\beta'}^{k\beta} \right. \\ &\quad \left. + (\mathcal{H}_{\text{int}}^2)_{k\beta}^{k\beta'} \delta_{\alpha}^{\alpha'} \right\} \\ &- \frac{1}{2} \left\{ (\langle\mathcal{H}_{\text{int}}\rangle^2)_{\alpha}^{\alpha'} \delta_{\beta}^{\beta'} - 2 \langle\mathcal{H}_{\text{int}}\rangle_{\alpha}^{\alpha'} \langle\mathcal{H}_{\text{int}}\rangle_{\beta}^{\beta'} \right. \\ &\quad \left. + (\langle\mathcal{H}_{\text{int}}\rangle^2)_{\beta}^{\beta'} \delta_{\alpha}^{\alpha'} \right\} \end{aligned} \quad (16)$$

Operator  $\Lambda$  contains essential information on the directions of coherence loss in both non-Markovian and Markovian systems, and  $-\Lambda$  is of the special form expected from a Lindblad dissipator to generate completely positive Markovian evolution. It has been implicitly defined previously (see, e.g., Refs. [40, 43, 47]) under the constraint of vanishing environmental average of the interaction ( $\langle\mathcal{H}_{\text{int}}\rangle = 0$ ), and typically occurs in conjunction with the interaction picture and the weak coupling limit [compare Eq. (4.14) in Ref. [40] with Eq. (17)]. Here, we have arrived at  $\Lambda$  for arbitrary interaction strength and without leaving the Schrödinger picture or requiring a vanishing bath average of the interaction (the latter point is

important for the inclusion of carrier-carrier scattering in nanostructures).

Up to the third order in time, Eq. (13) can now be approximated as

$$\rho_S(t) = e^{-i\mathcal{L}_{\text{eff}}t - \Lambda t^2 + o(t^3)}\rho_S(0) \quad (17)$$

where  $\mathcal{L}_{\text{eff}} \equiv \mathcal{L}_{\text{eff}}(0)$ . Now, on the time interval  $[0, \tau]$ , where according to our postulate  $\tau$  is shorter than any other relevant timescale in the problem, Eq. (17) should be valid. If we coarsen over this interval, we obtain

$$\frac{\rho_S(\tau) - \rho_S(0)}{\tau} = \left(-i\mathcal{L}_{\text{eff}} - \left.\frac{d\Gamma}{dt}\right|_{[0, \tau]}\right)\rho_S(0) \quad (18)$$

where

$$\left.\frac{d\Gamma}{dt}\right|_{[0, \tau]} = \frac{\int_0^\tau 2\Lambda t dt}{\tau} = \Lambda\tau$$

Since the memory is reset after each  $\tau$ , we can partition the time axis into intervals of length  $\tau$ ,  $t_n = n\tau$ , so that the environment is assumed to interact with the system in exactly the same way during each interval  $[t_n, t_{n+1}]$ .<sup>52, 55</sup> Resetting of memory means  $\Gamma(t_n^+) = \Gamma(0^+) = 0$ , after which  $\Gamma$  again starts evolving quadratically as  $\Gamma(t \in [t_n^+, t_{n+1}^-]) = \Lambda(t - t_n)^2$ . On this interval,

$$\left.\frac{d\Gamma}{dt}\right|_{[t_n, t_{n+1}]} = \frac{\int_{t_n^+}^{t_{n+1}^-} 2\Lambda(t - t_n) dt}{\tau} = \Lambda\tau$$

Moreover, due to the memory loss at  $t_n$ , the “initial” system state for the evolution on  $[t_n^+, t_{n+1}^-]$  becomes  $\rho_{S,n} = \rho_S(t_n)$ . As a result

$$\begin{aligned} \frac{\rho_{S,n+1} - \rho_{S,n}}{\tau} &= \left(-i\mathcal{L}_{\text{eff}} - \left.\frac{d\Gamma}{dt}\right|_{[t_n, t_{n+1}]}\right)\rho_{S,n} \\ &= (-i\mathcal{L}_{\text{eff}} - \Lambda\tau)\rho_{S,n} \end{aligned} \quad (19)$$

The term on the left approximates the first derivative, so the system’s evolution over  $\tau$  results in a completely positive Markovian dynamical map

$$\frac{d\rho_S}{dt} = (-i\mathcal{L}_{\text{eff}} - \Lambda\tau)\rho_S(t) \quad (20)$$

The nonzero eigenvalues of  $\Lambda$ , multiplied by  $\tau$ , define a set of new characteristic times for the system evolution, and for the Markovian approximation to be consistent, it must hold<sup>47</sup>  $\lambda\tau^2 \ll 1$ , where  $\lambda$  is the largest eigenvalue of  $\Lambda$  (which can be very large for bosonic environments). *The eventual steady state must clearly be a density matrix belonging to  $\mathcal{N}(\mathcal{L}_{\text{eff}}) \cap \mathcal{N}(\Lambda)$ , the intersection of the null-spaces of  $\mathcal{L}_{\text{eff}}$  and  $\Lambda$ .* Therefore, one can pinpoint the steady state as the component of the initial state belonging to  $\mathcal{N}(\mathcal{L}_{\text{eff}}) \cap \mathcal{N}(\Lambda)$ . The steady state does not depend on the actual value of  $\tau$ ; the existence of an ultrashort (but nonzero!)  $\tau$  was important to be able to utilize the short time expansion of the exact evolution to the shortest order. Once the coarse-graining was justified, the actual value of  $\tau$  is irrelevant as long as we are only interested in what the steady state is, but not in how long it takes to get to it.

### 2.3. Reality Check: Two Simple Examples

On the following two simple examples we will answer the two most important questions that arise about the use of Eq. (20):

- (1) Is the time  $\tau$  really as short as we claim?
- (2) Will we indeed obtain relaxation towards the *correct* steady state?

The first question will be answered on the example of an exactly solvable model—the spin-boson Hamiltonian with pure dephasing, on which we can actually calculate  $\tau$  and show it is ultrashort. The second question will be answered by showing proper relaxation on both the spin-boson model and the Jaynes-Cummings Hamiltonian, used to describe relaxation of an excited atom in the presence of a thermal bath of photons of resonant energy. Questions 1 and 2 are answered more formally in a forthcoming publication.<sup>50</sup>

#### 2.3.1. Spin-Boson Model with Pure Dephasing

One of the few analytically solvable<sup>52,56-60</sup> open system problems is that of a two-level system coupled to a dephasing-only boson bath, with the relevant Hamiltonians are given by

$$\begin{aligned} \mathcal{H}_S &= \frac{\omega}{2} \sigma_z, & \mathcal{H}_E &= \sum_{\bar{q}} \Omega_{\bar{q}} \left( b_{\bar{q}}^\dagger b_{\bar{q}} + \frac{1}{2} \right) \\ \mathcal{H}_{\text{int}} &= \sum_{\bar{q}} \sigma_z \{ g(\Omega_{\bar{q}}) b_{\bar{q}} + g(\Omega_{\bar{q}})^* b_{\bar{q}}^\dagger \} \end{aligned} \quad (21)$$

Here,  $\sigma_z$  is the Pauli matrix,  $b_{\bar{q}}^\dagger$  and  $b_{\bar{q}}$  and the boson creation and annihilation operators of the  $q$ -th boson mode, respectively,  $\pm\omega/2$  are the system energy levels (divided by  $\hbar$ ), and  $\Omega_{\bar{q}}$  is the boson mode frequency. The boson modes are initially in a thermal state with  $\langle n_{\bar{q}} \rangle = \langle b_{\bar{q}}^\dagger b_{\bar{q}} \rangle = 1/(\exp(\hbar\Omega_{\bar{q}}/k_B T) - 1)$ . Because of the interaction linear in environment creation/annihilation operators,  $\langle \mathcal{H}_{\text{int}} \rangle = 0$ , so  $\mathcal{L}_S = \mathcal{L}_{\text{eff}}$ , [see Eq. (15a)]:

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_S = \omega \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (22)$$

where the rows/columns are ordered as  $1 = |+\rangle\langle +|$ ,  $2 = |+\rangle\langle -|$ ,  $3 = |-\rangle\langle +|$ ,  $4 = |-\rangle\langle -|$  ( $\pm$  refer to the positive/negative (upper/lower) energy state). Operator  $\Lambda$  can be calculated according to (16) as

$$\Lambda = \lambda_d \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{aligned} \lambda_d &= 2 \sum_{\bar{q}} |g(\Omega_{\bar{q}})|^2 \coth \left( \frac{\hbar\Omega_{\bar{q}}}{2k_B T} \right) \\ &= 2 \int_0^\infty d\Omega \mathcal{D}(\Omega) |g(\Omega)|^2 \coth \left( \frac{\hbar\Omega}{2k_B T} \right) \end{aligned} \quad (23)$$

where  $\mathcal{D}(\Omega)$  is the density of boson states.

$\mathcal{L}_S$  and  $\Lambda$  obviously commute, and their common zero eigenspace [ $\mathcal{N}(\Lambda) = \mathcal{N}(\mathcal{L}_{\text{eff}})$ ] contains all density matrices with zero off-diagonal elements. This means that, for a given initial density matrix, the off-diagonal matrix elements will decay to zero while the diagonal elements remain unchanged:

$$\begin{aligned} [\rho_S(t)]_{++} &= [\rho_S(0)]_{++}, & [\rho_S(t)]_{--} &= [\rho_S(0)]_{--} \\ [\rho_S(t)]_{+-} &= [\rho_S(0)]_{+-} e^{-i\omega t - \lambda_d \tau t}, & [\rho_S(t)]_{-+} &= [\rho_S(0)]_{-+} e^{+i\omega t - \lambda_d \tau t} \end{aligned}$$

The steady state will be determined by simply annulling the off-diagonal elements. This is the correct steady state, as shown in the exact solution.<sup>47</sup>

The decoherence exponent  $\Gamma(t)$  in the exact solution behaves as

$$\Gamma(t) = \int_0^\infty d\Omega 2\mathcal{D}(\Omega) |g(\Omega)|^2 \coth \left( \frac{\hbar\Omega}{2k_B T} \right) \frac{\sin^2(\Omega t/2)}{(\Omega/2)^2} \quad (24)$$

For short-times,  $\Gamma(t) \approx \lambda_d t^2$ , as should be expected, because we know our expansion (17) is exact up to the second order in time. In the long-time limit for  $\Gamma(t)$ , only the low frequency contributions survive, since  $\lim_{t \rightarrow \infty} \sin^2(\Omega t/2)/(\Omega/2)^2 t = 2\pi\delta(\Omega)$ , so

$$\Gamma(t \rightarrow \infty) = t \lim_{\Omega \rightarrow 0} 2\pi \mathcal{D}(\Omega) |g(\Omega)|^2 \coth \left( \frac{\hbar\Omega}{2k_B T} \right) \quad (25)$$

We need to match this long-time behavior of  $\Gamma(t)$  with our coarse-grained term  $\lambda_d \tau t$ , in order to obtain  $\tau$ .

$$\tau = \lim_{t \rightarrow \infty} \frac{\Gamma(t)}{\lambda_d t} = \frac{\lim_{\Omega \rightarrow 0} 2\pi \mathcal{D}(\Omega) |g(\Omega)|^2 \coth(\hbar\Omega/2k_B T)}{2 \int_0^\infty d\Omega \mathcal{D}(\Omega) |g(\Omega)|^2 \coth(\hbar\Omega/2k_B T)} \quad (26)$$

Let us consider the example of an Ohmic bath (e.g., page 228 of Ref. [47]), with  $\mathcal{D}(\Omega) |g(\Omega)|^2 = (1/4)\Omega \exp(-\Omega/\Omega_c)$  and  $\Omega_c$  being a density-of-states cut-off frequency. Typically,  $\hbar\Omega_c \gg k_B T$ . In the numerator, one can approximate  $\coth(\hbar\Omega/2k_B T) \approx 2k_B T/\hbar\Omega$ , while the coth function in the denominator is always greater than 1, yielding

$$\tau < \left( \frac{k_B T}{\hbar\Omega_c} \right) \frac{2\pi}{\Omega_c} \ll \frac{2\pi}{\Omega_c}$$

Being typically the largest frequency scale in the full SE problem,  $\Omega_c$  sets the shortest physical timescale. Clearly,  $\tau$  is even shorter than the period associated with  $\Omega_c$ , which justifies our use of the short-time expansion and subsequent coarse-graining.

Note the long-time behavior  $\exp(-t/\tau_T)$  of the decoherence term  $\Gamma$ , where  $\tau_T = \hbar/\pi k_B T$  is the thermal correlation time. However, our time  $\tau$  is the *mathematical* coarse-graining time, which is very short. The relationship between the correct physical correlation loss time and the mathematically appropriate time is  $\lambda_d \tau \tau_T = 1$ .

### 2.3.2. Jaynes-Cummings Model in the Rotating Wave Approximation

The Jaynes-Cummings Hamiltonian in the rotating-wave approximation<sup>61-64</sup> describes the decay of a two-level system in the presence of a single boson mode of resonant frequency. The relevant Hamiltonians are

$$\begin{aligned} \mathcal{H}_S &= \frac{1}{2} \omega \sigma_z, & \mathcal{H}_E &= \omega \left( b^\dagger b + \frac{1}{2} \right) \\ \mathcal{H}_{\text{int}} &= g(b^\dagger \sigma_- + b \sigma_+) \end{aligned} \quad (27)$$

Here,  $\sigma_z$ ,  $\sigma_+ = (\sigma_x + i\sigma_y)/e$ , and  $\sigma_- = (\sigma_x - i\sigma_y)/2$  are the Pauli matrices,  $b^\dagger$  and  $b$  are the boson creation and annihilation operators, respectively,  $\pm\omega/2$  are the system energy levels (in units of frequency) and  $\omega$  is also the boson mode frequency, and  $g$  is a parameter measuring the interaction strength. The boson mode is initially in a thermal state with  $\langle n \rangle = \langle b^\dagger b \rangle = 1/(\exp(\hbar\omega/k_B T) - 1)$ . As in the spin-boson example,  $\mathcal{L}_{\text{eff}} = \mathcal{L}_S$  because of the interaction linear in environment creation/annihilation operators [see (15a)]:

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_S = \omega \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (28)$$

Operator  $\Lambda$  can be calculate according to Eq. (16) as

$$\Lambda = \frac{g^2}{2} \begin{bmatrix} 2\langle n \rangle + 2 & 0 & 0 & -2\langle n \rangle \\ 0 & 2\langle n \rangle + 1 & 0 & 0 \\ 0 & 0 & 2\langle n \rangle + 1 & 0 \\ -2\langle n \rangle - 2 & 0 & 0 & 2\langle n \rangle \end{bmatrix} \quad (29)$$

$\mathcal{L}_S$  and  $\Lambda$  commute, and we immediately note two common one-dimensional eigenspaces:  $\rho_{+-}$  is associated with the  $\mathcal{L}_S$  and  $\Lambda$  eigenvalues  $\omega$  and  $g^2(2\langle n \rangle + 1)/2$ , respectively, while  $\rho_{-+}$  is associated with the eigenvalues  $-\omega$  and  $g^2(2\langle n \rangle + 1)/2$ .

On the other hand, the space spanned by  $|+\rangle\langle+|$  and  $|-\rangle\langle-|$  is the null space of  $\mathcal{L}_{\text{eff}}$ . Solving the eigenproblem of  $\Lambda$  reduced to this space gives

$$\begin{aligned} \det \begin{bmatrix} g^2(\langle n \rangle + 1) - \lambda & -g^2\langle n \rangle \\ -g^2\langle n \rangle & g^2\langle n \rangle - \lambda \end{bmatrix} &= 0 \\ \lambda = 0 \quad \text{and} \quad \lambda &= \lambda_d \equiv g^2(2\langle n \rangle + 1) \end{aligned} \quad (30)$$

An eigenvector  $\mu^0 = (\mu_{++}^0, \mu_{--}^0)^T$  corresponding to the zero eigenvalue of the matrix  $\Lambda$  is characterized by

$$\mu_{--}^0 = \mu_{++}^0 \frac{\langle n \rangle + 1}{\langle n \rangle} \quad (31)$$

If we are looking for a density matrix that belongs to the zero eigenspace of  $\Lambda$ , it also has to satisfy the constraint of the unit trace, which fixes

$$\mu_{++}^0 = \frac{\langle n \rangle}{2\langle n \rangle + 1}, \quad \mu_{--}^0 = \frac{\langle n \rangle + 1}{2\langle n \rangle + 1} \quad (32)$$

One recognizes these components as the *thermal equilibrium values* of the population of the upper and lower level of our two-level system, respectively (see, for instance, p. 149 of Ref. [47]). Therefore, by seeking the steady state in  $\mathcal{N}(\Lambda) \cap \mathcal{N}(\mathcal{L}_{\text{eff}})$ , we have obtained the physically correct result.

## 3. THE RESONANT-TUNNELING DIODE (RTD)

A resonant-tunneling diode is a two-barrier tunneling structure. Typical dimensions of both the barriers and the well range from 2 to 5 nm. The barriers are usually AlGaAs, while the well is GaAs, all grown by MBE. RTD is a popular model system due to its pronounced quantum-mechanical features and one-dimensional transport. The best RTD transport results have been obtained using Wigner-function techniques.<sup>9, 10, 26, 65</sup>

The interaction between the active region and the contacts has so far been addressed within the model on the RTD as a two-level system, where the electron can either be in the RTD bound state (“+” state) or absent from the RTD (“-” state).<sup>66</sup> However, since the RTD naturally has open boundaries and continuous spectrum, as one finds in any quantum-mechanics textbook, the two-level models must usually be supplemented with a phenomenological resonance width to account for the fact that there are quite a few plane waves from the contact that contribute to the making of the bound state. Moreover, the continuum-state current increase after the valley cannot be captured by employing a two-level model for the RTD. The openness of the RTD active region has also been addressed in the works of Frensley<sup>26</sup> and Pötzt,<sup>28, 67</sup> as well as in the work of the Purdue group,<sup>18, 20, 21</sup> where the contacts are accounted for through a special injection self-energy term.<sup>68</sup>

A schematic of the simulated RTD under bias is given in Figure 2: the RTD well width is 3 nm, each barrier’s thickness is 5 nm, and the barrier height is 0.3 eV. The Fermi level in each contact is at 0.1 eV, below the equilibrium bound state, which is at 0.15 eV. A negative bias  $V$  is applied to the left contact, and, for simplicity, we will assume that all of the voltage drop occurs across the well and barriers. While still focusing on the active region/contacts interaction, we will offer an RTD model different from those previously



published. We will retain the wave picture in the RTD: for any given energy  $\mathcal{E}_k = \hbar^2 k^2 / 2m$  above the bottom of the higher, left contact, the single particle Hamiltonian of the RTD has doubly degenerate eigenfunctions: the forward-propagating state (not a plane wave!)  $\Psi_k$ , and the backward-propagating state  $\Psi_{-k}$ . These wavefunctions are not plane waves; rather, they are associated with plane waves being incident onto the barrier from the left and right contacts, respectively, and have the following behavior to the far left and right of the heterostructure:

$$\begin{aligned}\Psi_k(x \rightarrow -\infty) &= e^{ikx} + r_{-k,L} e^{-ikx} \\ \Psi_k(x \rightarrow +\infty) &= t_{k',R} e^{ik'x}\end{aligned}\quad (33a)$$

$$\begin{aligned}\Psi_{-k}(x \rightarrow +\infty) &= e^{-ik'x} + r_{k',R} e^{ik'x} \\ \Psi_{-k}(x \rightarrow -\infty) &= t_{-k,L} e^{-ikx}\end{aligned}\quad (33b)$$

where  $k$  and  $k'$  are the wavevectors in the left and right contact, respectively, that correspond to the same energy:  $k^2 = 2m\mathcal{E}_k/\hbar^2 = k'^2 - 2meV/\hbar^2$ . We will use  $k$  and  $-k$  associated with this energy to label the forward and backward propagating states, respectively, even though the backward propagating states are actually injected with  $+k'$ . The subscripts in the transmission and reflection coefficient denote the final wavevector and contact (for instance, reflected wave originally incident from the left with  $k$ , has the wavevector  $-k$  and remains in the contact  $L$ , thus notation  $r_{-k,L}$ ). What is important is that we adopt a potential profile (or, in numerical calculation, couple with a Poisson solver) that will enable us to solve for  $\Psi_k$  and  $\Psi_{-k}$  and find the transmission and reflection coefficients of the forward and backward propagating plane waves. Here, a simple linear potential drop across the well and barriers is adopted. Associated with  $\Psi_k$  ( $\Psi_{-k}$ ) in the active region are the creation and destruction operators  $d_k^\dagger$  and  $d_k$  ( $d_{-k}^\dagger$  and  $d_{-k}$ ), so that active region Hamiltonian is described by

$$\mathcal{H}_S = \sum_k \omega_k (d_k^\dagger d_k + d_{-k}^\dagger d_{-k}) \quad (34)$$

where  $\omega_k = \mathcal{E}_k/\hbar$ . It is important to note that the discussion in this section disregards the spin quantum number, which only adds to the degeneracy. The resulting currents at the end of the section should be considered “per spin orientation.”

In addition, the active region communicates with the reservoirs of charge—the contacts. We introduce a model interaction for the coupling between the eigenfunctions  $\Psi_k$  from the active region and the forward propagating plane waves, injected from the left contact and associated with the creation/annihilation operators  $c_{k,L}^\dagger$  and  $c_{k,L}$ , as well as the resulting transmitted and reflected waves (associated with  $c_{k',R}^\dagger/c_{k',R}$  and  $c_{-k,L}^\dagger/c_{-k,L}$ , respectively):

$$\begin{aligned}\mathcal{H}_{\text{int},+} &= \sum_{k>0} \Delta_L(k) \{ (c_{k,L}^\dagger + r_{-k,L}^* c_{-k,L}^\dagger) d_k \\ &+ d_k^\dagger (c_{k,L} + r_{-k,L} c_{-k,L}) \} \\ &+ \Delta_R(k') \{ t_{k',R}^* c_{k',R}^\dagger d_k + t_{k',R} d_k^\dagger c_{k',R} \}\end{aligned}\quad (35)$$

This model interaction is plausible for fully coherent transport, because we couple the states with the same energy only; no scattering from phonons will be included in this picture.  $\Delta_R$  and  $\Delta_L$  are the constants that in principle depend on the barrier thickness, accumulated charge near the RTD etc. For the time being, we will assume they are known. Similar to (35), the interaction of the backward-propagating waves, and the reflected and transmitted wave stemming from it, with the active region is given by:

$$\begin{aligned}\mathcal{H}_{\text{int},-} &= \sum_{k>0} \Delta_R(-k') \{ (c_{-k',R}^\dagger + r_{k',R}^* c_{k',R}^\dagger) d_{-k} \\ &+ d_{-k}^\dagger (c_{-k',R} + r_{k',R} c_{k',R}) \} \\ &+ \Delta_L(-k) \{ t_{-k,L}^* c_{-k,L}^\dagger d_{-k} + t_{-k,L} d_{-k}^\dagger c_{-k,L} \}\end{aligned}\quad (36)$$

When we put it all together, we have for the interaction Hamiltonian of the active region with the left/right contact:

$$\begin{aligned}\mathcal{H}_{\text{int},L} &= \sum_{k>0} \Delta_L(k) \{ (c_{k,L}^\dagger + r_{-k,L}^* c_{-k,L}^\dagger) d_k \\ &+ d_k^\dagger (c_{k,L} + r_{-k,L} c_{-k,L}) \} \\ &+ \Delta_L(-k) \{ t_{-k,L}^* c_{-k,L}^\dagger d_{-k} + t_{-k,L} d_{-k}^\dagger c_{-k,L} \}\end{aligned}\quad (37a)$$

$$\begin{aligned}\mathcal{H}_{\text{int},R} &= \sum_{k>0} \Delta_R(-k') \{ (c_{-k',R}^\dagger + r_{k',R}^* c_{k',R}^\dagger) d_{-k} \\ &+ d_{-k}^\dagger (c_{-k',R} + r_{k',R} c_{k',R}) \} \\ &+ \Delta_R(k') \{ t_{k',R}^* c_{k',R}^\dagger d_k + t_{k',R} d_k^\dagger c_{k',R} \}\end{aligned}\quad (37b)$$

Since all the interaction Hamiltonians are linear in the contact creation and destruction operators, and we assume that the initial states of the contacts are thermal-equilibrium grand-canonical ensembles,  $\langle \mathcal{H}_{\text{int},L/R} \rangle = 0$ . This means that  $\mathcal{L}_S = \mathcal{L}_{\text{eff}}$ , and also leaves us with only the first three terms in Eq. (16) for  $\Lambda$  to calculate. One can show that  $\Lambda = \Lambda_L + \Lambda_R$ , where

$$\begin{aligned}(\Lambda_{L/R})_{\alpha',\beta'}^{\alpha,\beta} &= \frac{1}{2} \left( \langle \mathcal{H}_{\text{int},L/R}^2 \rangle_{\alpha'}^{\alpha} \delta_{\beta'}^{\beta} + \langle \mathcal{H}_{\text{int},L/R}^2 \rangle_{\beta'}^{\beta} \delta_{\alpha'}^{\alpha} \right. \\ &\left. - 2 \sum_{i,j} \rho_{L,R}^i (\mathcal{H}_{\text{int},L/R})_{i\alpha'}^{j\alpha} (\mathcal{H}_{\text{int},L/R})_{j\beta'}^{i\beta} \right)\end{aligned}\quad (38)$$

The first and the second term in Eq. (38) give a general contribution of the form  $\Lambda_{\alpha\beta}^{\alpha\beta}$ , since

$$\begin{aligned}\langle \mathcal{H}_{\text{int},L}^2 \rangle &= \sum_{k>0} \Delta_L^2(k) \{ (\langle n_{k,L} \rangle + |r_{-k,L}|^2 \langle n_{-k,L} \rangle) d_k d_k^\dagger \\ &+ [(1 - \langle n_{k,L} \rangle) + (1 - \langle n_{-k,L} \rangle) |r_{-k,L}|^2] d_k^\dagger d_k \} \\ &+ \Delta_L(-k) \{ \langle n_{-k,L} \rangle |t_{-k,L}|^2 d_{-k} d_{-k}^\dagger \\ &+ (1 - \langle n_{-k,L} \rangle) |t_{-k,L}|^2 d_{-k}^\dagger d_{-k} \}\end{aligned}\quad (39)$$

preserves the filling of states.



In contrast, the third term in (38)

$$\begin{aligned} & \sum_{i,j} \rho_L^i (\mathcal{H}_{\text{int},L})_{i\alpha'}^{j\alpha} (\mathcal{H}_{\text{int},L})_{j\beta}^{i\beta'} \\ &= \sum_{k>0} \Delta_L^2(k) \{ [(1 - \langle n_{k,L} \rangle) \\ &+ (1 - \langle n_{-k,L} \rangle) |r_{-k,L}|^2] (d_k^\dagger)_\alpha (d_k^\dagger)_\beta \\ &+ [\langle n_{k,L} \rangle + \langle n_{-k,L} \rangle |r_{-k,L}|^2] (d_k^\dagger)_\alpha (d_k^\dagger)_\beta \} \\ &+ \Delta_L^2(-k) \{ [(1 - \langle n_{-k,L} \rangle) |t_{-k,L}|^2 (d_{-k}^\dagger)_\alpha (d_{-k}^\dagger)_\beta \\ &+ \langle n_{-k,L} \rangle |t_{-k,L}|^2 (d_{-k}^\dagger)_\alpha (d_{-k}^\dagger)_\beta \} \end{aligned} \quad (40)$$

gives a contribution of the form  $\Lambda_{\beta\beta}^{\alpha\alpha}$ .

Each term in  $\Lambda$  attacks only single particle states with a given  $k$ , so in reality we have a multitude of two-level problems, where the two levels are the particle being in  $k$  (“+”) and the particle being absent from  $k$  (“-”). In each of these 4-dimensional subspaces (see the two-level examples in Section 2.3),  $\mathcal{L}_S$  is zero in the space spanned by  $|+\rangle\langle+|$  and  $|-\rangle\langle-|$ , so to find the steady state we need to deal only with the diagonal components  $\rho_k^{++}$  and  $\rho_k^{--}$  which can be shown to obey

$$\frac{d\rho_k^{++}}{dt} = -a\rho_k^{++} + b\rho_k^{--} \quad (41a)$$

$$\frac{d\rho_k^{--}}{dt} = a\rho_k^{++} - b\rho_k^{--} \quad (41b)$$

where

$$\begin{aligned} a &= \tau \{ \Delta_L^2(k) [(1 - \langle n_{k,L} \rangle) + (1 - \langle n_{-k,L} \rangle) |r_{-k,L}|^2] \\ &+ \Delta_R^2(k') (1 - \langle n_{k',R} \rangle) |t_{k',R}|^2 \} \\ b &= \tau \{ \Delta_L^2(k) [\langle n_{k,L} \rangle + \langle n_{-k,L} \rangle |r_{-k,L}|^2] \\ &+ \Delta_R^2(k') \langle n_{k',R} \rangle |t_{k',R}|^2 \} \end{aligned} \quad (42)$$

Clearly,  $(d\rho_k^{++}/dt) + (d\rho_k^{--}/dt) = 0$ , as it should be, because  $\rho_k^{++} = \text{Tr}(\rho_S d_k^\dagger d_k) = f(k)$  and  $\rho_k^{--} = \text{Tr}(\rho_S d_k d_k^\dagger) = 1 - f(k)$ .

Therefore, we can write  $df(k)/dt = -(a+b)f(k) + b$ , so in the steady state  $f_\infty(k) = b/(a+b)$ . When written in the notation more common in transport  $\langle n_{\pm k,L/R} \rangle \equiv f_{L/R}(\pm k)$  (the Fermi distribution in the left/right contact), we obtain the steady-state distribution for the forward-propagating states  $\Psi_k$ :

$$\begin{aligned} f_\infty(k) &= \frac{b}{a+b} \\ &= \frac{\Delta_L^2(k) [f_L(k) + |r_{-k,L}|^2 f_L(-k)] + \Delta_R^2(k') f_R(k') |t_{k',R}|^2}{\Delta_L^2(k) (1 + |r_{-k,L}|^2) + \Delta_R^2(k') |t_{k',R}|^2} \end{aligned} \quad (43a)$$

Similarly, one obtains for the backward propagating states

$$\begin{aligned} f_\infty(-k) &= \frac{\Delta_R^2(-k') [f_R(-k') + |r_{k',R}|^2 f_R(k')] + \Delta_L^2(-k) f_L(-k) |t_{-k,L}|^2}{\Delta_R^2(-k') (1 + |r_{k',R}|^2) + \Delta_L^2(-k) |t_{-k,L}|^2} \end{aligned} \quad (43b)$$

In the simplest approximation,  $\Delta_L = \Delta_R = \Delta$ , and

$$f_\infty(k) = \frac{f_L(k) (1 + |r_{-k,L}|^2) + f_R(k') |t_{k',R}|^2}{1 + |r_{-k,L}|^2 + |t_{k',R}|^2} \quad (44a)$$

$$f_\infty(-k) = \frac{f_R(k') (1 + |r_{k',R}|^2) + f_L(k) |t_{-k,L}|^2}{1 + |r_{k',R}|^2 + |t_{-k,L}|^2} \quad (44b)$$

In equilibrium, we automatically obtain  $f_\infty(k) = f_\infty(-k) = f_L = f_R$ . Note how, *only if the transmission is low* do  $f_\infty(k) \rightarrow f_L(k)$  and  $f_\infty(-k) \rightarrow f_R(k')$ , which is the assumption most often used in mesoscopic calculations, but we see may not be entirely justified. If there is appreciable transmission, the active region feels the distributions in both contacts.

The current (per spin orientation) can be calculated according to the quantum-mechanical relationship

$$\begin{aligned} j_\infty(x) &= \frac{-e\hbar}{2mi} \sum_{k>0} f_\infty(k) \left[ \frac{d\Psi_k^*(x)}{dx} \Psi_k(x) \right. \\ &\quad \left. - \Psi_k^*(x) \frac{d\Psi_k(x)}{dx} \right] \|\Psi_k\|^{-2} \\ &+ f_\infty(-k) \left[ \frac{d\Psi_{-k}^*(x)}{dx} \Psi_{-k}(x) \right. \\ &\quad \left. - \Psi_{-k}^*(x) \frac{d\Psi_{-k}(x)}{dx} \right] \|\Psi_{-k}\|^{-2} \\ &= \sum_{k>0} f_\infty(k) j_k(x) + f_\infty(-k) j_{-k}(x) \end{aligned} \quad (45)$$

Each of the two current components, carried by the forward and backward propagating states, is constant across the structure. The simplest way to calculate them is by focusing on the regions far from the barriers, where the wavefunctions are plane waves. So to the far right of the heterostructure

$$\begin{aligned} j_\infty^+ &= \frac{-e\hbar}{2mi} \sum_{k>0} f_\infty(k) \frac{|t_{k,R}|^2 (2ik')}{\|\Psi_k\|^2} \\ &= \frac{-e\hbar}{m} \frac{W}{2\pi} \int_0^\infty dk f_\infty(k) \frac{|t_{k,R}|^2 k'}{\|\Psi_k\|^2} \end{aligned} \quad (46)$$

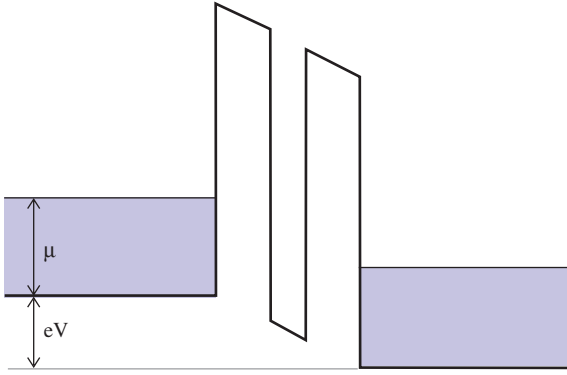
$$= \frac{-eW}{h} \int_0^\infty d\mathcal{E} f_\infty[k(\mathcal{E})] \frac{\mathcal{T}(\mathcal{E})}{\|\Psi_{k(\mathcal{E})}\|^2} \quad (47)$$

where we have used that  $|t(k,R)|^2 k'/k = \mathcal{T}(\mathcal{E})$ , the transmission coefficient that is the same for both directions and a function of energy only, and  $k dk = m d\mathcal{E}/\hbar^2$ . Also,  $W$  is the total width of the active region (the well, the barriers, and a large enough portion of the contacts to get to the flat band condition). Similarly, the current component (per spin) carried by the backward propagating states can be found as

$$j_\infty^- = \frac{eW}{h} \int_0^\infty d\mathcal{E} f_\infty[-k(\mathcal{E})] \frac{\mathcal{T}(\mathcal{E})}{\|\Psi_{-k(\mathcal{E})}\|^2} \quad (48)$$

so the total current (per spin orientation) can be found as

$$j_\infty = \frac{-eW}{h} \int_0^\infty d\mathcal{E} \left( \frac{f_\infty[k(\mathcal{E})]}{\|\Psi_{k(\mathcal{E})}\|^2} - \frac{f_\infty[-k(\mathcal{E})]}{\|\Psi_{-k(\mathcal{E})}\|^2} \right) \mathcal{T}(\mathcal{E}) \quad (49)$$

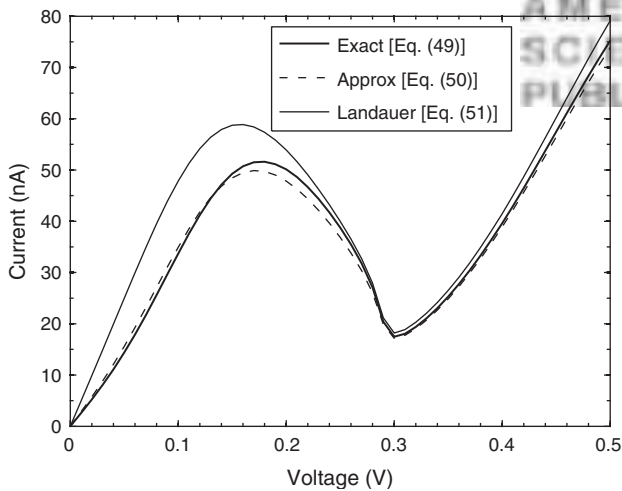


**Fig. 2.** Schematic of a resonant-tunneling diode under bias. The barrier thickness in the simulated device is 5 nm, the well width 3 nm, and the barrier height 0.3 eV. For simplicity, the voltage drop is assumed to occur completely across the well and barriers. The Fermi level  $\mu$  in each contact is taken to be 0.1 eV, located below the bound state in equilibrium, which is at 0.15 eV.

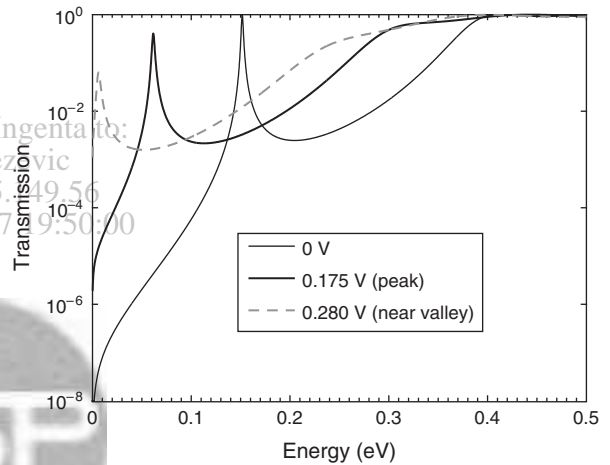
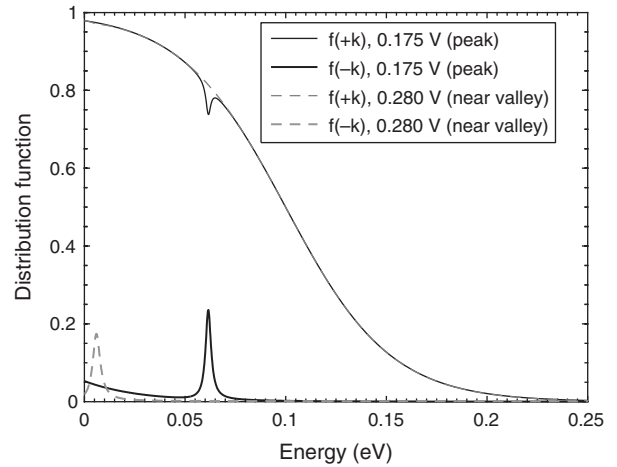
Note that this expression is completely parameter-free, and  $\|\Psi_{\pm k}\|^2$  in the denominator scale as  $\sim W$ . Namely, in the case we take a very large portion of each contact as part of the active region, then  $\|\Psi_{\pm k}\|^2 \approx (1 + |r_{\pm k}|^2)W/2 + |t_{\pm k}|^2W/2 = W/2[2 - \mathcal{F}(\mathcal{E}) + \mathcal{F}(\mathcal{E})(\mathcal{E}/(\mathcal{E} + eV))^{\pm 1/2}]$ . Therefore, the current can be approximated as

$$j_{\infty}^{\text{approx}} = \frac{-2e}{h} \int_0^{\infty} d\mathcal{E} \left( \frac{f_L(\mathcal{E})[2 - \mathcal{F}(\mathcal{E})] + f_R(\mathcal{E} + eV)\mathcal{F}(\mathcal{E})(\mathcal{E}/(\mathcal{E} + eV))^{1/2}}{[2 - \mathcal{F}(\mathcal{E}) + \mathcal{F}(\mathcal{E})(\mathcal{E}/(\mathcal{E} + eV))^{1/2}]^2} - \frac{f_R(\mathcal{E} + eV)[2 - \mathcal{F}(\mathcal{E})] + f_L(\mathcal{E})\mathcal{F}(\mathcal{E})(\mathcal{E}/(\mathcal{E} + eV))^{-1/2}}{[2 - \mathcal{F}(\mathcal{E}) + \mathcal{F}(\mathcal{E})(\mathcal{E}/(\mathcal{E} + eV))^{-1/2}]^2} \right) \mathcal{F}(\mathcal{E}) \quad (50)$$

Figure 3 shows the I–V curve of the RTD from Figure 2, as calculated according to the exact expression (49), the approximate formula (50), and the Landauer formula for



**Fig. 3.** Steady state I–V curve for the RTD of Figure 2, according to the exact expression (49) (bold solid curve), the approximate formula (50) (dashed curve), and the Landauer formula (51) (thin solid curve). Landauer formula predicts a much higher peak current and a lower peak voltage, because it does not account for the distribution functions’ deviation from the contact equilibrium distributions (see Fig. 4), which is important near transmission peaks.



**Fig. 4.** (Top panel) Steady-state distribution for the forward [ $f(+k)$ ] and backward [ $f(-k)$ ] propagating states, at the peak voltage (0.175 V) and very near the valley voltage (0.28 V). Note significant deviations from the Fermi-Dirac equilibrium distributions in the leads, which coincide with the transmission peaks in the bottom panel (Note: energy scales in the two panels are different). (Bottom panel) Transmission coefficient in equilibrium, at the peak voltage (0.175 V), and very near the valley (0.28 V) of the I–V curve in Figure 3. As the voltage increases, the transmission peak corresponding to the bound state decreases in magnitude and shifts towards lower energies, eventually vanishing at the valley bias.

the current per spin orientation

$$j_{\infty}^L = \frac{-e}{h} \int_0^{\infty} d\mathcal{E} [f_L(\mathcal{E}) - f_R(\mathcal{E} + eV)] \mathcal{F}(\mathcal{E}) \quad (51)$$

The width of each contact that is considered part of the active region is 20 times the width of the well and barriers combined. We see that the Landauer formula (51) predicts the peak at a lower voltage and significantly overestimates the peak current with respect to the exact solution (49). The reason is that the distribution functions for the forward and backward propagating states (top panel of Fig. 4) coincide with the distribution functions for the left and right reservoirs only where the transmission is not high. There are significant deviations in these distribution functions from the reservoir Fermi-Dirac distribution functions, which coincide with the transmission peak

energies (bottom panel of Fig. 4)—a transmitting nanostructure feels the Fermi distributions in *both contacts*. Both (49) and (51) describe ballistic transport, so no crossing of the curves typical for the inclusion of inelastic scattering should be expected. The only difference between (49) and (51) is that (49) captures the pronounced nonlocal nature of tunneling. The agreement between the approximate expression (50) and the exact solution (49) is clearly very good.

#### 4. SUMMARY AND CONCLUDING REMARKS

This work described the formalism that is capable of capturing the decoherence in quasiballistic nanodevices, occurring due to the active region-contact interaction, as the principal mechanism that governs relaxation. Starting from the non-Markovian dynamics of an abstract open system, we first showed that the long-time Markovian behavior can be obtained through coarse-graining of the exact evolution over ultrashort times. This enabled us to obtain Markovian relaxation, and consequently identify the proper steady state, directly from first principles (the details of the microscopic Hamiltonians and the state of the environment). The steady state must belong to the intersection of the null spaces of an effective system Liouvillian and a dissipative operator  $\Lambda$ , quadratic in the interaction. Using the presented approach, we obtained the proper equilibrium state on the examples of the spin-boson model with pure dephasing and the Jaynes-Cummings Hamiltonian. Finally, the problem of a ballistic resonant-tunneling diode was addressed in detail. We explicitly calculated the steady state distributions of the forward and backward propagating states, and showed that, when the transmission through the structure is high, the active region “feels” the distributions in both contacts. The nonequilibrium distribution functions actually have peaks/dips at the energies corresponding to transmission maxima. The resulting steady-state  $I$ - $V$  curve shows the prominent resonant features without any free parameters, with a higher peak voltage and lower peak current than predicted by the Landauer formula. This work will hopefully contribute to the understanding of decoherence and relaxation in nanodevices, and facilitate the exploitation of the open system techniques in quantum transport theory.

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