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Optical master equations for quantum transport of hot electrons

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Abstract. Using ideas of Herbert and Till, analogues of discrete energy levels of electrons in quantum optics are introduced into quantum transport theory. For simple one-dimensional devices inelastic scattering with optical phonons is modelled by a reservoir. A master equation is derived following the usual procedures in quantum optics. The hot electron kinetic equation of Herbert, with corrections, is deduced as a first approximation. Our formalism is applied to a simplified tunnelling diode structure.

1. Introduction

Boltzmann equations are primarily used for the description of transport in semiconductor devices [1]. In this approach it is assumed that an electron suffers many spatially localized collisions during the transit through the device, and each collision is temporally separated from another. Moreover, the collision rates are regarded as independent of driving fields. For sub-micron devices it is expected that these assumptions will begin to break down, and quantum effects will be important. Collisions become non-local in space and time and strong driving fields can accelerate the electrons during collisions. Herbert [2], some years ago, following Till and Herbert [3] obtained quantum kinetic equations which were comparatively simple to analyse and gave reasonable agreement [4] with numerical solutions. Optical phonon scattering was treated only in a relaxational approximation. In this paper we will obtain a master equation for the single-particle density matrix in a device with a driving field and inelastic phonon scattering using the concept of 'trajectories' introduced by Herbert. First we will summarize the approach of Herbert to quantum kinetic equations.

The trajectory method, as developed by Herbert, can be derived from a Schrödinger equation [2] or Boltzmann equation [4] approach. An electron trajectory represents a classical energy level accessible to the current flow across the device being modelled. A classical trajectory is quantum mechanically represented by a wavepacket. Differential equations can be written which include both the effects of scattering between trajectories and of reflection and interference from voltage structures. For our purposes it is convenient to write the equations for a one-dimensional device as

$$\frac{\mathrm{d}}{\mathrm{d}t}q_{tr}(x) = -\frac{\partial}{\partial x}j_{tr}(x) - S_{\mathrm{o}}(x)\,q_{tr}(x) + S_{tr+1,tr}(x)\,q_{tr+1}(x) + S_{tr-1,tr}(x)\,q_{tr-1}(x) \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}j_{tr} = -S_{\mathrm{o}}(x)\,j_{tr} - \langle v\rangle(x)\,\frac{\partial}{\partial x}\left(\langle v\rangle(x)\,q_{tr}(x)\right) \tag{2}$$

where $S_{tr,tr+1}$, for example, is the scattering rate from trajectory tr into trajectory $tr+1$, S_o is the total scattering out of the trajectory tr, and $\langle v \rangle$ is a quantity called the local velocity. q_{tr} and j_{tr} are the average charge and current, respectively, associated with the trajectory. The local velocity is the ratio of current to charge for the wavepackets representing the trajectory. The local velocity does not properly take into account the effects of scattering. The master equation approach that we will give deals with this scattering quite rigorously.

It can be seen immediately that these equations can form a powerful modelling tool. They consist of first-order ordinary differential equations, whose stability and numerical properties are well established. They can be solved much faster and more easily than complete density-matrix, Boltzmann equation or Monte Carlo techniques, while still being able to adequately represent electron overshoot [4] and other hot-electron effects in various microstructures of interest [5].

In figure 1 the trajectories (which can be considered as wavepackets around stationary energy states of the free particle in a step-like potential) are separated by $\hbar\omega$, the energy of an optical phonon. In a practical calculation we can consider a finite ladder of trajectories. Approximate analytic solutions are then possible within each region [4] and the regions can be matched numerically.

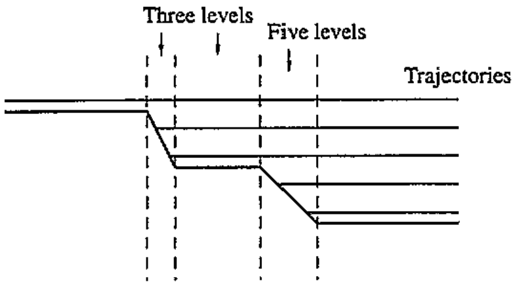

Figure 1. Trajectory ladders used to analyse a device.

2. The master equation

We will consider our system of carriers coupled to a large heat bath of optical phonons with a single energy ω. The system is one-dimensional with a space-dependent voltage but no magnetic field. Coulombic electron–electron interactions are ignored. The electron–phonon coupling is taken to be momentum-independent, which is a common approximation to the Fröhlich Hamiltonian [6]. The Hamiltonian $\mathcal{H}$ for the system therefore has the form

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_{SB} \tag{3}$$

with

$$\mathcal{H}_S = \sum_E E\mathcal{A}_E^\dagger \mathcal{A}_E \tag{4}$$

$$\mathcal{H}_B \approx \sum_k \omega C_k^\dagger C_k \tag{5}$$

and

$$\mathcal{H}_{SB} = \gamma \sum_{l,k} \left(\mathcal{A}_{l+k}^\dagger \mathcal{A}_l C_k + \mathcal{A}_{l-k}^\dagger \mathcal{A}_l C_k^\dagger \right). \tag{6}$$

The $\mathcal{A}_E$ are electron annihilation operators for the energy eigenstates of the one-particle Hamiltonian $\mathcal{H}^{(1)}$,

$$\mathcal{H}^{(1)} = \tfrac{1}{2}\hat{p}^2 + V(\hat{x}) \tag{7}$$

where $V(x)$ represents the voltage profile in the device; $\hat{p}$ and $\hat{x}$ are the single-particle momentum and position operators, respectively. The $\mathcal{A}_l$ are electron annihilation operators associated with momentum eigenstates. C_k is the phonon annihilation operator of momentum k. We can characterize the bath by an average particle number $\bar{n}$ and a decay constant η so that

$$\langle C_k^\dagger(t)\, C_{k'}(t')\rangle_{\mathrm{B}} = \delta_{kk'}\mathrm{e}^{-\eta|t-t'|}\mathrm{e}^{\mathrm{i}\omega(t-t')}\bar{n} \tag{8}$$

and

$$\langle C_k^\dagger(t)\, C_{k'}^\dagger(t')\rangle_{\mathrm{B}} = \langle C_k(t)\, C_{k'}(t')\rangle_{\mathrm{B}} = 0\,. \tag{9}$$

(Here the subscript B denotes a bath average.) As usual [7, 8] we will assume that γ is small and the bath is large so that (8) and (9) hold at all times. Consequently it is a good approximation in the interaction picture to write the total density matrix as

$$\rho^{\mathrm{I}}(t) = \rho_{\mathrm{S}}^{\mathrm{I}}(t)\, \rho_{\mathrm{B}}^{\mathrm{I}}(0) \tag{10}$$

where $\rho_{\mathrm{B}}^{\mathrm{I}}(0)$ is the time-independent bath density matrix. The standard formula for the Markovian evaluation [8] of the reduced density matrix $\rho_{\mathrm{S}}^{\mathrm{I}}(t)$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}^{\mathrm{I}}(t) = -\int_0^t \mathrm{Tr_B}\left[\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t)\,,\left[\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t'),\, \rho_{\mathrm{S}}^{\mathrm{I}}(t)\,\rho_{\mathrm{B}}^{\mathrm{I}}\right]\right]\mathrm{d}t'\,. \tag{11}$$

($t = 0$ is the time that the interaction is switched on.)

Noting that

$$\mathcal{A}_l = \int \mathrm{d}x\, \langle l|x\rangle \mathcal{A}_x = \int \mathrm{d}x\, \frac{\mathrm{e}^{-\mathrm{i}lx}}{\sqrt{2\pi}}\mathcal{A}_x \tag{12a}$$

and

$$\mathcal{A}_x = \sum_E \langle x|E\rangle \mathcal{A}_E \tag{12b}$$

we can rewrite $\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}$ as

$$\begin{aligned}\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}} = \gamma \sum_{E_0 E_1} \int \mathrm{d}x\, \mathrm{e}^{\mathrm{i}(E_0-E_1)t}\mathcal{A}_{E_0}^\dagger \langle E_0|x\rangle\langle x|E_1\rangle \mathcal{A}_{E_1} \\ \times \sum_k \left(\mathrm{e}^{\mathrm{i}kx}C_k{}^I(t) + \mathrm{e}^{-\mathrm{i}kx}C_k^{\dagger I}(t)\right)\end{aligned} \tag{13}$$

where $|E_0\rangle$ and $|E_1\rangle$ are eigenstates of $\mathcal{H}^{(1)}$ with eigenvalues E_0 and E_1, respectively. From (11) we can transform back to the Schrödinger picture through

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = -\mathrm{i}\,[\mathcal{H}_{\mathrm{S}}, \rho_{\mathrm{S}}] + \left(\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}^{\mathrm{I}}\right)_{\mathrm{I}\longrightarrow \mathrm{S}}\,. \tag{14}$$

Using (12b) and the results of appendix A,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}} = -\mathrm{i}\,[\mathcal{H}_{\mathrm{S}}, \rho_{\mathrm{S}}] + 2\pi\gamma^2 \sum_{E_0 E_1} \int \mathrm{d}x \Bigg\{ -\mathcal{A}_x^\dagger \mathcal{A}_x \mathcal{A}_{E_0}^\dagger \langle x|E_0\rangle\langle E_0|x\rangle\langle x|E_1\rangle \mathcal{A}_{E_1}\rho_{\mathrm{S}} \\ \times\left[(\bar{n}+1)\left[\pi\delta(E_0 - E_1 + \omega) - \frac{\mathrm{i}\mathcal{P}}{E_0 - E_1 + \omega}\right]\right.\end{aligned}$$

$$+\bar{n}\left[\pi\delta(E_0-E_1-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_0-E_1-\omega}\right]\Bigg]$$

$$+\mathcal{A}_x^\dagger\mathcal{A}_x\rho_S\mathcal{A}_{E_0}^\dagger\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}$$

$$\times\Bigg[\bar{n}\left[\pi\delta(E_0-E_1+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_0-E_1+\omega}\right]$$

$$+(\bar{n}+1)\left[\pi\delta(E_0-E_1-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_0-E_1-\omega}\right]\Bigg]$$

$$+\text{ Hermitian conjugate}\Bigg\}. \tag{15}$$

This is a many-particle density matrix. In order to derive the trajectory equations of Herbert we need to obtain an effective master equation for a single-particle density matrix $\rho^{(1)}(x,x')$. To each creation operator we will associate a ket for the analogous one-particle state, e.g.,

$$\mathcal{A}_k^\dagger\mathcal{A}_j\longrightarrow|k\rangle\langle j| \tag{16}$$

and so we will define

$$\rho^{(1)}=\sum_{j,k}\mathrm{Tr}\big(\mathcal{A}_j^\dagger\mathcal{A}_k\rho_S\big)\,|k\rangle\langle j|\,. \tag{17}$$

($|k\rangle$ could be $|x\rangle$ or $|E\rangle$ here.)

We have the consistency check that

$$\mathrm{Tr}\big(\mathcal{A}_j^\dagger\mathcal{A}_k\rho_S\big)=\mathrm{Tr}\big(|j\rangle\langle k|\,\rho^{(1)}\big)\,. \tag{18}$$

From equation (17) we derive

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{kj}^{(1)}=\mathrm{Tr}\left(\mathcal{A}_j^\dagger\mathcal{A}_k\frac{\mathrm{d}}{\mathrm{d}t}\rho_S\right). \tag{19}$$

We will write the canonical anticommutation relations as

$$\big\{\mathcal{A}_i^\dagger,\mathcal{A}_j\big\}=\langle j|i\rangle\,. \tag{20}$$

We note that

$$\mathcal{A}_i^\dagger\mathcal{A}_j\mathcal{A}_l^\dagger\mathcal{A}_m=\mathcal{A}_i^\dagger\mathcal{A}_m\langle j|l\rangle-\mathcal{A}_i^\dagger\mathcal{A}_l^\dagger\mathcal{A}_j\mathcal{A}_m \tag{21}$$

and

$$\big[\mathcal{A}_i^\dagger\mathcal{A}_j,\mathcal{A}_l^\dagger\mathcal{A}_m\big]=\mathcal{A}_i^\dagger\mathcal{A}_m\langle j|l\rangle-\mathcal{A}_l^\dagger\mathcal{A}_j\langle m|i\rangle\,. \tag{22}$$

Now we will consider the contribution of the Hamiltonian term in (15)–(19). $\mathcal{H}_S$ is a one-body Hamiltonian and so can be written in the form

$$\mathcal{H}_S=\sum_{l,m}\mathcal{A}_l^\dagger\mathcal{A}_mH_{lm}\,. \tag{23}$$

The relevant contribution is

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^{(1)}=-\mathrm{i}\sum_{k,j}\mathrm{Tr}\big(\mathcal{A}_j^\dagger\mathcal{A}_k\,[\mathcal{H}_S,\rho_S]\big)\,|k\rangle\langle j|$$

$$=-\mathrm{i}\sum_{k,j}\mathrm{Tr}\big(\big[\mathcal{A}_j^\dagger\mathcal{A}_k,\mathcal{H}_S\big]\rho_S\big)\,|k\rangle\langle j|\,. \tag{24}$$

On using (22) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^{(1)}=-\mathrm{i}\big[\mathcal{H}^{(1)},\rho^{(1)}\big]. \tag{25}$$

This argument is further developed in appendix A and from (A6*d*) we deduce

$$\frac{d\rho^{(1)}}{dt} = -i[\mathcal{H}^{(1)}, \rho^{(1)}] + 2\pi\gamma^2 \sum_{E_2,E_3} \int dx \Big\{ - |x\rangle \langle x|E_2\rangle\langle E_2|x\rangle\langle x|E_3\rangle \langle E_3| \rho^{(1)}$$
$$\times \Big[(\bar{n}+1) \Big[\pi\delta(E_2 - E_3 + \omega) - \frac{i\mathcal{P}}{E_2 - E_3 + \omega} \Big]$$
$$+ \bar{n} \Big[\pi\delta(E_2 - E_3 - \omega) - \frac{i\mathcal{P}}{E_2 - E_3 - \omega} \Big] \Big]$$
$$+ |x\rangle \langle x| \rho^{(1)} |E_2\rangle \langle E_2|x\rangle\langle x|E_3\rangle \langle E_3|$$
$$\times \Big[\bar{n} \Big[\pi\delta(E_2 - E_3 + \omega) - \frac{i\mathcal{P}}{E_2 - E_3 + \omega} \Big]$$
$$+ (\bar{n}+1) \Big[\pi\delta(E_2 - E_3 - \omega) - \frac{i\mathcal{P}}{E_2 - E_3 - \omega} \Big] \Big] + \text{Hermitian conjugate} \Big\}$$
$$+ 2\pi\gamma^2 \sum_{E_0,E_1,E_2,E_3} \int dx \Big[\Big[\pi\delta(E_2 - E_3 - \omega) - \frac{i\mathcal{P}}{E_2 - E_3 - \omega} \Big]$$
$$- \Big[\pi\delta(E_2 - E_3 + \omega) - \frac{i\mathcal{P}}{E_2 - E_3 + \omega} \Big] \Big]$$
$$\{ |E_1\rangle \langle x|E_3\rangle \langle E_1 E_3| \rho^{(2)} |x E_2\rangle \langle E_2|x\rangle\langle x|E_0\rangle \langle E_0|$$
$$- |E_1\rangle \langle E_1|x\rangle\langle x|E_3\rangle \langle x E_3| \rho^{(2)} |E_0 E_2\rangle \langle E_2|x\rangle \langle E_0| \} \tag{26}$$

where

$$\langle E_1 E_3| \rho^{(2)} |x E_2\rangle = \mathrm{Tr}\big(\rho_S \mathcal{A}^{\dagger}_{E_2} \mathcal{A}^{\dagger}_{x} \mathcal{A}_{E_3} \mathcal{A}_{E_1}\big) \tag{27}$$

and $\rho^{(2)}$ represents a part of ρ_S which cannot be represented by $\rho^{(1)}$, and it is customary to ignore it. The derivation given in this section is quite a conventional one for obtaining Markov master equations and will be useful for comparisons with the trajectory method.

3. The trajectory master equation

We will give a heuristic discussion of the trajectory concept for the sake of clarity. Not all the degrees of freedom of the bath space $\mathcal{B}$ in the last section will be treated as bath variables. $\mathcal{B}$ can be decomposed as

$$\mathcal{B} = \bigoplus_{n=0}^{\infty} \mathcal{B}_n \tag{28}$$

where $\mathcal{B}_n$ is the space of n-phonon states. For $\mathcal{B}$ to be a bath we consider large energies for $\mathcal{B}$:

$$\mathcal{B}_n \approx \{ |E = n\omega, v\rangle : v \in \mathcal{B}' \} . \tag{29}$$

Here $\mathcal{B}'$ represents degrees of freedom in $\mathcal{B}$ which lead at most to a dressed energy shift much less than $\hbar\omega$. As a particularly pertinent example different distributions of momentum of phonons may lead to the same total energy. Since part of the bath degrees of freedom will be incorporated into the system, we will denote the modified system by $\mathcal{S}'$. The modified system kets will be written in the form $|x, tr\rangle$ or $|E\sigma, tr\rangle$ (depending on the electron basis).

The overall state space becomes

$$\Psi \approx \begin{cases} \{|E_{\rm B}, x\rangle\} \bigotimes \mathcal{B}' \\ \text{or} \\ \{|E_{\rm B}, E\sigma\rangle\} \bigotimes \mathcal{B}' \end{cases} \tag{30}$$

and

$$E_{\rm B} = E_0 + \omega\, tr \tag{31}$$

where tr is the 'trajectory' integer. The convention is that the trajectory of highest electron energy under consideration is represented by $tr = 0$. We can now write the Hamiltonian corresponding to $\mathcal{S}'$ and its interaction with $\mathcal{B}'$. The modified system Hamiltonian is

$$\mathcal{H}_{\rm S'} = \sum_{E\sigma} \sum_{tr} (E + E_0 + \omega\, tr)\, |E\sigma, tr\rangle\, \langle E\sigma, tr| \,. \tag{32}$$

The interaction part of the Hamiltonian is

$$\mathcal{H}_{\rm S'B'} = \gamma \sum_{l,k} \sum_{tr} \left(|l+k, tr-1\rangle\, \langle l, tr|\, C'_k + |l-k, tr\rangle\, \langle l, tr-1|\, C'^{\dagger}_k \right). \tag{33}$$

As before the bath correlations will be taken to satisfy

$$\left\langle C'^{\dagger}_k(t)\, C'_{k'}(t') \right\rangle_{\rm B'} = \delta_{kk'} {\rm e}^{-\eta|t-t'|} \bar{n} \tag{34a}$$

$$\left\langle C'^{\dagger}_k(t)\, C'^{\dagger}_{k'}(t') \right\rangle_{\rm B'} = \left\langle C'_k(t)\, C'_{k'}(t') \right\rangle_{\rm B'} = 0 \,. \tag{34b}$$

In the interaction representation

$$\mathcal{H}^{\rm I}_{\rm S'B'} = \gamma \sum_{tr} \sum_{E\sigma} \sum_{E'\sigma'} \sum_{k} \int {\rm d}x\, {\rm e}^{{\rm i}(E-E')t} \times \Big\{ |E\sigma, tr-1\rangle\, \langle E\sigma|x\rangle \langle x|E'\sigma'\rangle \left\langle E'\sigma', tr\right| {\rm e}^{{\rm i}kx} C'^{\rm I}_k {\rm e}^{-{\rm i}\omega t} + |E\sigma, tr\rangle\, \langle E\sigma|x\rangle \langle x|E'\sigma'\rangle \left\langle E'\sigma', tr-1\right| {\rm e}^{-{\rm i}kx} C'^{\dagger {\rm I}}_k {\rm e}^{{\rm i}\omega t} \Big\} . \tag{35}$$

The master equation analogous to (11) is

$$\frac{\rm d}{{\rm d}t} \rho^{\rm I}_{\rm S'}(t) = -\int_0^t {\rm Tr}_{\rm B'} \left[\mathcal{H}^{\rm I}_{\rm S'B'}(t)\,, \left[\mathcal{H}^{\rm I}_{\rm S'B'}(t'),\, \rho^{\rm I}_{\rm S'}(t)\, \rho^{\rm I}_{\rm B'} \right]\right] {\rm d}t' \,. \tag{36}$$

From equation (35) it is straightforward to show that the assumption that $\rho^{\rm I}_{\rm S'}$ is diagonal in the 'tr' space is consistent with (36). From now on we will make this assumption, which is reasonable since tr is a bath degree of freedom of $\mathcal{B}$, and so we can write

$$\rho_{\rm S'} = \sum_{tr} \rho_{tr}\, |tr\rangle\, \langle tr| \,. \tag{37}$$

Using appendix B we can deduce that in the Schrödinger representation

$$\frac{\rm d}{{\rm d}t} \rho_{tr} = -{\rm i}\, [\mathcal{H}_{\rm S'}, \rho_{tr}] + 2\pi\gamma^2 \sum_{E\sigma} \sum_{E'\sigma'} \int {\rm d}x \Bigg\{ -|x\rangle\, \langle x|E\sigma\rangle \langle E\sigma|x\rangle \langle x|E'\sigma'\rangle \langle E'\sigma'|\rho_{tr} \times \left[(\bar{n}+1) \left[\pi\delta(E - E' + \omega) - \frac{{\rm i}\mathcal{P}}{E - E' + \omega} \right] + \bar{n} \left[\pi\delta(E - E' - \omega) - \frac{{\rm i}\mathcal{P}}{E - E' - \omega} \right] \right] + |x\rangle\, \langle x|\, \rho_{tr+1}\, |E\sigma\rangle\, \langle E\sigma|x\rangle \langle x|E'\sigma'\rangle \langle E'\sigma'|$$

$$\times\bar{n}\left[\pi\delta\big(E-E'+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'+\omega}\right]$$
$$+\,|x\rangle\,\langle x|\,\rho_{tr-1}\,|E\sigma\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|$$
$$\times\,(\bar{n}+1)\left[\pi\delta\big(E-E'-\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'-\omega}\right]+\text{Hermitian conjugate}\Bigg\}. \tag{38}$$

The density matrix for the unmodified system is obtained by tracing over the trajectory and

$$\rho_{\mathrm{S}}=\sum_{tr}\rho_{tr}\,. \tag{39}$$

From equation (38) we can deduce that ρ_{S} satisfies (26).

4. The trajectory equations

We will now further simplify the evolution equation for ρ_{tr}. On excluding scattering into the trajectory we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{tr}\Big|_{\text{No inward scattering}}=-\mathrm{i}\,[\mathcal{H}_{\mathrm{S}'},\rho_{tr}]+2\pi\gamma^2\sum_{E\sigma}\sum_{E'\sigma'}\int\mathrm{d}x$$
$$\times\Bigg\{-|x\rangle\langle x|E\sigma\rangle\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|\rho_{tr}$$
$$\times\Bigg[(\bar{n}+1)\left[\pi\delta\big(E-E'+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'+\omega}\right]$$
$$+\bar{n}\left[\pi\delta\big(E-E'-\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'-\omega}\right]\Bigg]$$
$$-\rho_{tr}|E'\sigma'\rangle\langle E'\sigma'|x\rangle\langle x|E\sigma\rangle\langle E\sigma|x\rangle\,\langle x|$$
$$\times\Bigg[(\bar{n}+1)\left[\pi\delta\big(E-E'+\omega\big)+\frac{\mathrm{i}\mathcal{P}}{E-E'+\omega}\right]$$
$$+\bar{n}\left[\pi\delta\big(E-E'-\omega\big)+\frac{\mathrm{i}\mathcal{P}}{E-E'-\omega}\right]\Bigg]\Bigg\}$$
$$=\;-\mathrm{i}\,[\mathcal{H}_{\mathrm{S}'},\rho_{tr}]+\sum_{E'\sigma'}\int\mathrm{d}x\big\{-|x\rangle\,\langle x|E'\sigma'\rangle f(x,E')\langle E'\sigma'|\rho_{tr}$$
$$-\rho_{tr}\,\big|E'\sigma'\big\rangle\,f^*(x,E')\langle E'\sigma'|x\rangle\,\langle x|\,\big\}$$
$$=\;-\mathrm{i}\,[\mathcal{H}_{\mathrm{S}'},\rho_{tr}]+\int\mathrm{d}x\Big\{-|x\rangle\,\langle x|\,f(x,\mathcal{H}_{\mathrm{S}'})\,\rho_{tr}-\rho_{tr}f^*(x,\mathcal{H}_{\mathrm{S}'})\,|x\rangle\,\langle x|\Big\} \tag{40}$$

where

$$f(x,E')=2\pi\gamma^2\sum_{E\sigma}\langle x|E\sigma\rangle\langle E\sigma|x\rangle\Bigg[(\bar{n}+1)\left[\pi\delta\big(E-E'+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'+\omega}\right]$$
$$+\bar{n}\left[\pi\delta\big(E-E'-\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E-E'-\omega}\right]\Bigg]. \tag{41}$$

If the energies contributing to ρ_{tr} are narrowly centred around E_{tr} then we can approximate f by the truncated Taylor series

$$f(x,\mathcal{H}_{\mathrm{S}'})\approx f(x,E_{tr})+\left[\frac{\partial f}{\partial E}(x,E_{tr})\right](\mathcal{H}_{\mathrm{S}'}-E_{tr})\,. \tag{42}$$

This approximation would not be good in a potential structure such as a quantum well where the function is not smoothly varying. For the descending staircase structure of figure 1, this is not a problem.

In order to recover the Herbert-like trajectory equations, it suffices to take $f(x, \mathcal{H}_{S'}) \approx f(x, E_{tr})$. On using this approximation (40) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{tr} = -\mathrm{i}\big(\mathcal{H}_{\mathrm{eff}}\rho_{tr} - \rho_{tr}\mathcal{H}^{\dagger}_{\mathrm{eff}}\big) \tag{43}$$

with

$$\mathcal{H}_{\mathrm{eff}} = \tfrac{1}{2}\hat{p}^2 + \big(V - E_{\mathrm{shift}} - \tfrac{1}{2}\mathrm{i}S_{\mathrm{o}}\big)(\hat{x}) \tag{44}$$

$$E_{\mathrm{shift}}(x) = \sum_{E\sigma} 2\pi\gamma^2 \Big\{ (\bar{n}+1)\frac{\mathcal{P}}{E - E_{tr} + \omega}\langle x|E\sigma\rangle\langle E\sigma|x\rangle + \bar{n}\frac{\mathcal{P}}{E - E_{tr} - \omega}\langle x|E\sigma\rangle\langle E\sigma|x\rangle\Big\} \tag{45}$$

$$S_{\mathrm{o}}(x) = \sum_{\sigma} 4\pi^2\gamma^2\big\{ (\bar{n}+1)\langle x|E_{tr+1}\sigma\rangle\langle E_{tr+1}\sigma|x\rangle + \bar{n}\langle x|E_{tr-1}\sigma\rangle\langle E_{tr-1}\sigma|x\rangle\big\}. \tag{46}$$

Owing to the Hermiticity of S_{o}, $\mathcal{H}_{\mathrm{eff}}$ itself is not Hermitian and so incorporates dissipation. We will now consider the other terms in the evolution which represent scattering into the trajectory:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho_{tr}(x,x')\Big|_{\text{Inwards scattering}} = 2\pi\gamma^2\sum_{E\sigma}\sum_{E'\sigma'}\Big\{ &\langle x|\rho_{tr+1}|E\sigma\rangle\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle\\ &\times\bar{n}\Big[\pi\delta\big(E - E' + \omega\big) - \frac{\mathrm{i}\mathcal{P}}{E - E' + \omega}\Big]\\ &+\langle x'|E\sigma\rangle\langle E\sigma|\rho_{tr+1}|x'\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle\\ &\times\bar{n}\Big[\pi\delta\big(E - E' + \omega\big) + \frac{\mathrm{i}\mathcal{P}}{E - E' + \omega}\Big]\\ &+\langle x|\rho_{tr-1}|E\sigma\rangle\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle\\ &\times(\bar{n}+1)\Big[\pi\delta\big(E - E' - \omega\big) - \frac{\mathrm{i}\mathcal{P}}{E - E' - \omega}\Big]\\ &+\langle x'|E\sigma\rangle\langle E\sigma|\rho_{tr-1}|x'\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle\\ &\times(\bar{n}+1)\Big[\pi\delta\big(E - E' - \omega\big) + \frac{\mathrm{i}\mathcal{P}}{E - E' - \omega}\Big]\Big\}.\end{aligned} \tag{47}$$

Now $\langle x|\rho_{tr}|E\sigma\rangle$ is strongly peaked at $E = E_{tr}$ and so

$$\begin{aligned}\sum_{E\sigma}\langle x|\rho_{tr-1}|E\sigma\rangle\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle(\bar{n}+1)\Big[\pi\delta\big(E - E' - \omega\big) - \frac{\mathrm{i}\mathcal{P}}{E - E' - \omega}\Big]\\ \approx \langle x|\rho_{tr-1}|x\rangle\langle x|E'\sigma'\rangle\langle E'\sigma'|x'\rangle(\bar{n}+1)\\ \times\Big[\pi\delta\big(E_{tr-1} - E' - \omega\big) - \frac{\mathrm{i}\mathcal{P}}{E_{tr-1} - E' - \omega}\Big].\end{aligned} \tag{48}$$

Hence

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho_{tr}(x,x')\Big|_{\text{Inwards scattering}} &\approx 2\pi\gamma^2\big\{q_{tr+1}(x)\,\bar{n}g_{tr}(x,x') + q_{tr+1}(x')\bar{n}g^*_{tr}(x,x')\\ &\quad+q_{tr-1}(x)(\bar{n}+1)g_{tr}(x,x') + q_{tr-1}(x')(\bar{n}+1)g^*_{tr}(x,x')\big\}\\ &\equiv \mathcal{I}(x,x')\end{aligned} \tag{49}$$

where

$$g_{tr}(x,x') = \sum_{E\sigma} \langle x|E\sigma\rangle\langle E\sigma|x'\rangle \left[\pi\delta(E_{tr}-E) - \frac{\mathrm{i}\mathcal{P}}{E_{tr}-E}\right] \tag{50}$$

and

$$q_{tr}(x) = \langle x|\,\rho_{tr}\,|x\rangle \tag{51}$$

where q_{tr} is the trajectory charge density that we introduced earlier. Our treatment will be valid provided the electrons are removed quickly enough that the exclusion principle is insignificant.

We have now the essential dynamical equation to derive (1) and (2):

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} q_{tr}(x)\,\Big|_{\text{No inward scattering}} &= -\mathrm{i}\,\langle x|\left(\mathcal{H}_{\mathrm{eff}}\rho_{tr} - \rho_{tr}\mathcal{H}^{\dagger}_{\mathrm{eff}}\right)|x\rangle \\
&= -\mathrm{i}\,\langle x|\,\tfrac{1}{2}\left(\hat{p}^2\rho_{tr} - \rho_{tr}\hat{p}^2\right)|x\rangle \\
&\quad -\mathrm{i}\,(V(x) - E_{\mathrm{shift}}(x))\,\langle x|\,\rho_{tr}\,|x\rangle - \mathrm{i}\,\langle x|\,\rho_{tr}\,|x\rangle\,(V(x) - E_{\mathrm{shift}}(x)) \\
&\quad -\tfrac{1}{2}S_{\mathrm{o}}(x)\,\langle x|\,\rho_{tr}\,|x\rangle - \langle x|\,\rho_{tr}\,|x\rangle\,\tfrac{1}{2}S_{\mathrm{o}}(x) \\
&= -\mathrm{i}\tfrac{1}{2}\,\langle x|\left[\hat{p},\left(\hat{p}\rho_{tr} + \rho_{tr}\hat{p}\right)\right]|x\rangle - S_{\mathrm{o}}(x)\,q_{tr}(x) \\
&= -\frac{\partial}{\partial x}\tfrac{1}{2}\langle x|\left(\hat{p}\rho_{tr} + \rho_{tr}\hat{p}\right)|x\rangle - S_{\mathrm{o}}(x)\,q_{tr}(x) \\
&= -\frac{\partial}{\partial x} j_{tr}(x) - S_{\mathrm{o}}(x)\,q_{tr}(x)\ .
\end{aligned} \tag{52}$$

The influence of scattering into the trajectory is given by

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} q_{tr}(x)\,\Big|_{\text{Inwards scattering}} &= 2\pi^2\gamma^2\left\{q_{tr+1}(x)\,\bar{n}\left(g_{tr}(x,x) + g^*_{tr}(x,x)\right)\right. \\
&\quad \left. + q_{tr-1}(x)\,(\bar{n}+1)\left(g_{tr}(x,x) + g^*_{tr}(x,x)\right)\right\} \\
&= q_{tr+1}(x)\,S_{tr+1,tr}(x) + q_{tr-1}(x)\,S_{tr-1,tr}(x)\ .
\end{aligned} \tag{53}$$

where

$$S_{tr,tr'}(x) = 4\pi^2\gamma^2 \sum_{\sigma} \langle x|E_{tr'}\sigma\rangle\langle E_{tr'}\sigma|x\rangle\left\{\bar{n}\delta_{tr-1,tr'} + (\bar{n}+1)\right\}\ . \tag{54}$$

Combining (52) and (54) we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} q_{tr}(x) &= -\frac{\partial}{\partial x} j_{tr}(x) - S_{tr,tr+1}(x)\,q_{tr}(x) - S_{tr,tr-1}(x)\,q_{tr}(x) \\
&\quad + S_{tr+1,tr}(x)\,q_{tr+1}(x) + S_{tr-1,tr}(x)\,q_{tr-1}(x)
\end{aligned} \tag{55}$$

which coincides with (1) on identifying $S_{\mathrm{o}}(x)$ with $S_{tr,tr+1}(x) + S_{tr,tr-1}(x)$.

The evaluation of $\mathrm{d}j/\mathrm{d}t$ is less straightforward than that of $\mathrm{d}q/\mathrm{d}t$. From (43) we know that the scattering out of the trajectory can be represented by a non-Hermitian Hamiltonian, $\mathcal{H}_{\mathrm{eff}}$. By linearity it is sufficient to consider a term of the form

$$\rho = |E_{\mathrm{eff}}\rangle\,\langle E'_{\mathrm{eff}}| \tag{56}$$

where

$$\mathcal{H}_{\mathrm{eff}}\,|E_{\mathrm{eff}}\rangle = E\,|E_{\mathrm{eff}}\rangle \tag{57a}$$

and

$$\langle E'_{\mathrm{eff}}|\mathcal{H}_{\mathrm{eff}} = \langle E'_{\mathrm{eff}}|E' \tag{57b}$$

(since the density matrix can be written as a sum of such terms). Hence in the absence of scattering into the trajectory

$$j(x) = \tfrac{1}{2} \langle x| \left(\hat{p} \, |E_{\text{eff}}\rangle \langle E'_{\text{eff}}| + |E_{\text{eff}}\rangle \langle E'_{\text{eff}}| \hat{p}\right) |x\rangle \tag{58}$$

and

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} j(x) &= \tfrac{1}{2} \langle x| \left\{ \hat{p} \left(-\mathrm{i}E \, |E_{\text{eff}}\rangle\right) \langle E'_{\text{eff}}| + \cdots \right\} |x\rangle \\ &= -\mathrm{i}(E - E')j(x) \,. \end{aligned} \tag{59}$$

Similarly from (51)

$$\frac{\mathrm{d}}{\mathrm{d}t} q(x) = -\mathrm{i}(E - E')q(x) \,. \tag{60}$$

By definition the effective velocity $\langle v \rangle$ is

$$\langle v \rangle(x) = \frac{j(x)}{q(x)} \,. \tag{61}$$

Hence, for no inward scattering,

$$\frac{\partial}{\partial x} \langle v \rangle \, q = \frac{\partial j}{\partial x} = -\frac{\mathrm{d}}{\mathrm{d}t} q - S_o q \tag{62}$$

on using (55). So

$$\begin{aligned} \langle v \rangle \frac{\partial}{\partial x} \langle v \rangle \, q &= \langle v \rangle \left[\mathrm{i}(E - E')q - S_o q \right] \\ &= \mathrm{i}(E - E')j - S_o j \\ &= -\frac{\mathrm{d}}{\mathrm{d}t} j - S_o j \,. \end{aligned} \tag{63}$$

In order for (61) to hold for an arbitrary density matrix, it is necessary that $\langle v \rangle$ is approximately independent of E and E' within the trajectory wavepacket.

To find $\langle v \rangle$ exactly it is necessary to solve the kinetic equations for the adjacent trajectories and apply (49) to determine the wavepacket present. Since the kinetic equations depend on $\langle v \rangle$ and are, in general, interdependent, this is not a trivial operation.

The simplest semi-classical approximation, appropriate if the correlation lengths are small compared to the device structure, is to take $\langle v \rangle = \sqrt{2E}$ similar to Herbert's time-dependent work [9].

The approximation most closely equivalent to Herbert [2] is to take $\langle v \rangle$ from (61) for the effective eigenstates (using appropriate boundary conditions). This allows for reflection from the device structure when interference effects are significant and, in this case, the suppression of interference caused by inelastic scattering.

Now

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} j_{tr} \Big|_{\text{Inwards scattering}} &= -\mathrm{i}\tfrac{1}{2} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)_{x'=x} \frac{\mathrm{d}}{\mathrm{d}t} \rho\left(x, x'\right) \\ &= -\mathrm{i}\pi\gamma^2 \Bigg\{ \frac{\partial q_{tr+1}}{\partial x} \bar{n} g_{tr}(x,x) + q_{tr+1} \bar{n} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)_{x'=x} g_{tr}(x,x') \\ &\qquad - \frac{\partial q_{tr+1}}{\partial x} \bar{n} g^*_{tr}(x,x) + q_{tr+1} \bar{n} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)_{x'=x} g^*_{tr}(x,x') + \cdots \Bigg\} \\ &= -2\pi\mathrm{i}\gamma^2 \Bigg\{ -\mathrm{i} \frac{\partial q_{tr+1}}{\partial x} \bar{n} \sum_{E\sigma} \langle x|E\sigma\rangle \langle E\sigma|x\rangle \frac{\mathcal{P}}{E_{tr} - E} \\ &\qquad + \pi q_{tr+1} \bar{n} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)_{x'=x} \langle x|E_{tr}\sigma\rangle \langle E_{tr}\sigma|x'\rangle + \cdots \Bigg\} \,. \end{aligned} \tag{64}$$

The term

$$\pi q_{tr+1}\bar{n}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)_{x'=x}\langle x|E_{tr}\sigma\rangle\langle E_{tr}\sigma|x'\rangle$$

vanishes since it is the total current for the energy subspace E_{tr} which is always zero because, for any eigenstate, the conjugate eigenstate always has exactly opposite current. Consequently,

$$S_{\rm bias}\equiv\frac{\mathrm{d}}{\mathrm{d}t}j_{tr}\Big|_{\rm Inwards\ scattering}=-2\pi\gamma^2\left\{\frac{\partial q_{tr+1}}{\partial x}\bar{n}+\frac{\partial q_{tr-1}}{\partial x}(\bar{n}+1)\right\}$$
$$\times\left\{\sum_{E\sigma}\langle x|E\sigma\rangle\langle E\sigma|x\rangle\frac{\mathcal{P}}{E_{tr}-E}\right\}. \qquad (65)$$

Collecting together terms we have from (63) and (65)

$$\frac{\mathrm{d}}{\mathrm{d}t}j_{tr}=-S_{\rm o}(x)\,j_{tr}-\langle v\rangle(x)\,\frac{\partial}{\partial x}\,\langle v\rangle(x)\,q_{tr}(x)-S_{\rm bias}(x)\ . \qquad (66)$$

The term (65) represents a preference for scattered electrons to travel in a particular direction due to interference effects. It is unlikely to make a qualitative difference to the model for two reasons: firstly, in more general cases there are similar classical terms [4] associated with momentum dependence in the electron–phonon interaction. Secondly, it is a principal-part expression caused by the part of (50) which represents non-energy conserving interactions that cause the wavepacket of energy states in the target trajectory to broaden; that is, it is of similar order to terms already neglected. Nevertheless, it does not add greatly to the complexity of the model and so has been retained. It may then be included or neglected when solving particular problems as appropriate. The same comments apply to the energy shifts (45) which are another very similar term often neglected in traditional calculations of this type in quantum optics.

5. Separating the left-bound and right-bound electron flow

We will now consider, as a concrete example, an extremely simplified resonant tunnelling diode structure such as that shown in figure 2.

The local velocity for any given energy is determined by calculating the eigenstates. It immediately becomes clear that there are two distinct solutions at each energy level, one associated with each scattering state. This suggests that it is more appropriate to solve for $q^{\rm L}_{tr}$ and $q^{\rm R}_{tr}$ than for q and j.

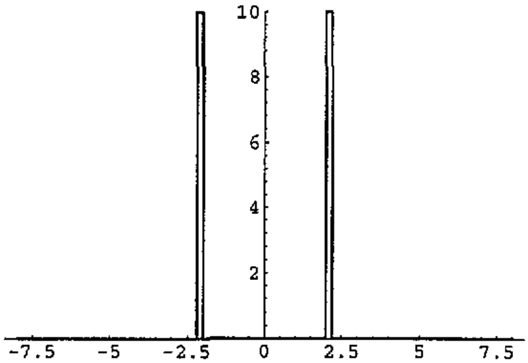

Figure 2. Voltage versus position.

Equations (55) and (66) become

$$0 = +\frac{\partial}{\partial x} v_{tr}^{\mathrm{L}} q_{tr}^{\mathrm{L}} - S_{\mathrm{o}} q_{tr}^{\mathrm{L}} + S_{\mathrm{in}}^{\mathrm{L}} \tag{67}$$

$$0 = -\frac{\partial}{\partial x} v_{tr}^{\mathrm{R}} q_{tr}^{\mathrm{R}} - S_{\mathrm{o}} q_{tr}^{\mathrm{R}} + S_{\mathrm{in}}^{\mathrm{R}} \tag{68}$$

where

$$S_{\mathrm{in}}^{\mathrm{L}} + S_{\mathrm{in}}^{\mathrm{R}} = S_{\mathrm{in}} \equiv q_{tr+1} S_{tr+1,tr} + q_{tr-1} S_{tr-1,tr} \,. \tag{69}$$

We still need to determine $S_{\mathrm{in}}^{\mathrm{L}}$ and $S_{\mathrm{in}}^{\mathrm{R}}$. Consider scattering from a single point, $S_{\mathrm{in}}^{\mathrm{Greens}} = S_{\mathrm{in}}\delta(x - x_0)$ and $S_{\mathrm{bias}}^{\mathrm{Greens}} = S_{\mathrm{bias}}\delta(x - x_0)$.

If we consider a small region around x_0 and ignore electrons entering this region from outside we can apply the classical approximation to (66), which for a steady-state solution is

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t} j_{tr} \\ &= -S_{\mathrm{o}}(x)\, j_{tr}(x) - k(x)\, \frac{\partial}{\partial x} k(x)\, q_{tr}(x) + S_{\mathrm{bias}}(x)\, \delta(x - x_0) \end{aligned} \tag{70}$$

where

$$k(x) = \sqrt{2(V(x) - E_{tr})}\,. \tag{71}$$

There is a discontinuity in q_{tr} at x_0 whose magnitude Δq_{tr} can be determined by taking the coefficient of $\delta(x - x_0)$ in (70):

$$0 = -k(x_0)^2\, \Delta q_{tr}(x_0) + S_{\mathrm{bias}}(x_0)\,. \tag{72}$$

Although we have ignored electrons entering the small region from the outside, the expression for $\Delta q_{tr}(x_0)$ is still valid since for any boundary condition the homogenous steady-state solution of q_{tr} is continuous.

Returning to the representation given by (67) and (68) we write

$$0 = +\frac{\partial}{\partial x} v_{tr}^{\mathrm{L}} q_{tr}^{\mathrm{L}} - S_{\mathrm{o}} q_{tr}^{\mathrm{L}} + S_{\mathrm{in}}^{\mathrm{L}} \delta(x - x_0) \tag{73}$$

$$0 = -\frac{\partial}{\partial x} v_{tr}^{\mathrm{R}} q_{tr}^{\mathrm{R}} - S_{\mathrm{o}} q_{tr}^{\mathrm{R}} + S_{\mathrm{in}}^{\mathrm{R}} \delta(x - x_0) \tag{74}$$

and taking the coefficient of the delta function gives

$$0 = v_{tr}^{\mathrm{L}}(x_0)\, \Delta q_{tr}^{\mathrm{L}}(x_0) + S_{\mathrm{in}}^{\mathrm{L}}(x_0) \tag{75}$$

$$0 = -v_{tr}^{\mathrm{R}}(x_0)\, \Delta q_{tr}^{\mathrm{R}}(x_0) + S_{\mathrm{in}}^{\mathrm{R}}(x_0)\,. \tag{76}$$

Now applying $\Delta q_{tr} = \Delta q_{tr}^{\mathrm{L}} + \Delta q_{tr}^{\mathrm{R}}$ we find

$$\frac{S_{\mathrm{bias}}}{k^2} = \frac{-S_{\mathrm{in}}^{\mathrm{L}}}{v_{tr}^{\mathrm{L}}} + \frac{S_{\mathrm{in}}^{\mathrm{R}}}{v_{tr}^{\mathrm{R}}} \tag{77}$$

so

$$S_{\mathrm{in}}^{\mathrm{R}} = \frac{v_{tr}^{\mathrm{R}} S_{\mathrm{in}}}{v_{tr}^{\mathrm{R}} + v_{tr}^{\mathrm{L}}} + \frac{v_{tr}^{\mathrm{R}} v_{tr}^{\mathrm{L}}}{k^2\left(v_{tr}^{\mathrm{R}} + v_{tr}^{\mathrm{L}}\right)} S_{\mathrm{bias}} \tag{78}$$

$$S_{\mathrm{in}}^{\mathrm{L}} = \frac{v_{tr}^{\mathrm{L}} S_{\mathrm{in}}}{v_{tr}^{\mathrm{R}} + v_{tr}^{\mathrm{L}}} - \frac{v_{tr}^{\mathrm{R}} v_{tr}^{\mathrm{L}}}{k^2\left(v_{tr}^{\mathrm{R}} + v_{tr}^{\mathrm{L}}\right)} S_{\mathrm{bias}}\,. \tag{79}$$

As previously discussed, it is probably a reasonable approximation to set $S_{\mathrm{bias}} = 0$ which simplifies these expressions considerably.

The derived steady-state equations are

$$-\frac{\partial}{\partial x}v_{tr}^{L}q_{tr}^{L} = -S_o q_{tr}^{L} + S_{in}^{L} \tag{80}$$

$$+\frac{\partial}{\partial x}v_{tr}^{R}q_{tr}^{R} = -S_o q_{tr}^{R} + S_{in}^{R} \tag{81}$$

where

$$v_{tr}^{R} = \frac{j_R}{q_R} = \mathrm{Im}\left\{\frac{\psi_R'}{\psi_R}\right\} \tag{82}$$

for the scattering state travelling to the right, and

$$v_{tr}^{L} = \frac{-j_L}{q_L} = -\mathrm{Im}\left\{\frac{\psi_L'}{\psi_L}\right\} \tag{83}$$

for the scattering state travelling to the left.

6. Numerical results

Figure 3 shows the transmission of the junction, without scattering, for energies from 2 to 3 units (as usual, we are working in units in which $\hbar$ and the electron's effective mass are both 1). The downwards slope to the right of the peak is related to the negative differential resistance typical of resonant tunnelling diodes. Over a wider energy range, more resonant energy peaks can be seen (figure 4).

Figures 5 and 6 show the transmission over the same energy range for relatively low and high scattering rates, respectively. The dots are the points calculated numerically. Figure 7 shows the three graphs superimposed.

Specifically, $4\pi^2\gamma^2$ is 0.2 in figure 5 and 0.8 in figure 6. $\bar{n} = 0.3$ and $\omega = 0.3$ in both cases. It is important to note that neither these figures nor the voltage profile are intended to represent any device currently existing; they were chosen essentially at random to demonstrate the general features of this technique. Only two trajectories (the trajectory at the base energy and one ω higher) were considered; the calculation was done using *Mathematica* [10], balancing the demands of efficiency and clarity. In practical calculations, much better results could be obtained using more carefully optimized code.

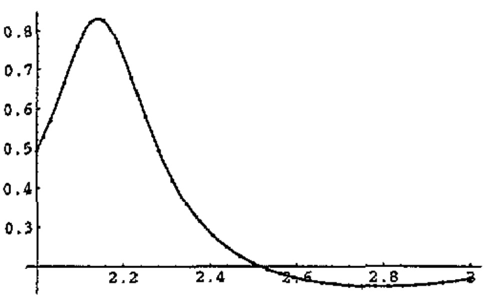

Figure 3. Transmission versus energy in the absence of scattering.

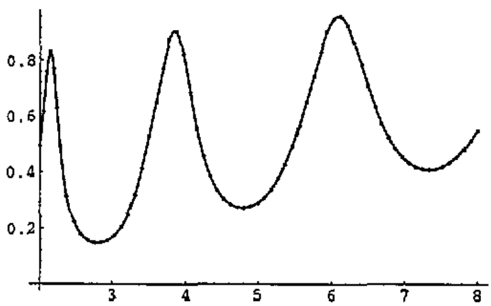

Figure 4. Transmission versus energy in the absence of scattering.

The most critical omission from the calculation is that no attempt was made to calculate a self-consistant solution including the mean-field electromagnetic electron–electron interaction.

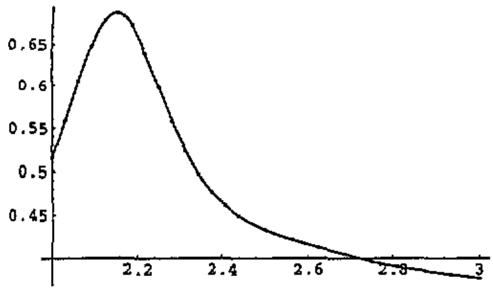

Figure 5. Transmission versus energy with light scattering.

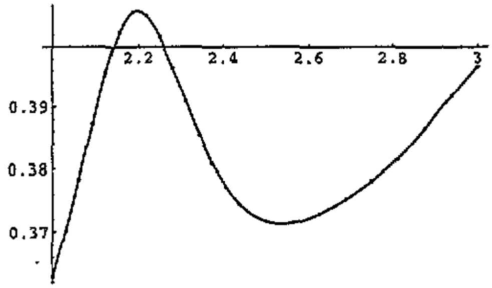

Figure 6. Transmission versus energy with heavy scattering.

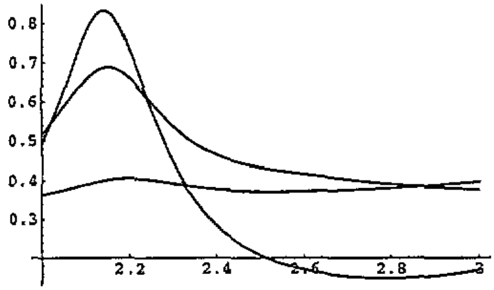

Figure 7. Transmission versus energy figures superimposed.

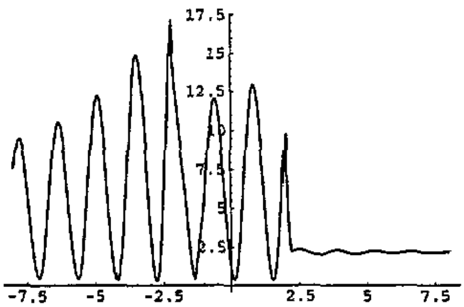

Figure 8. v_0^R versus position.

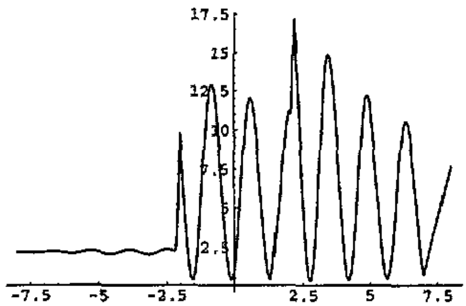

Figure 9. v_0^L versus position.

Figure 7 shows that in the absence of scattering, a strong interference effect is present. This depends on significant numbers of electrons being reflected between the barriers several times without losing coherence; as scattering is increased, this becomes impossible and the interference pattern is flattened out.

6.1. Charge distribution

We choose a single point on figure 5, $E = 2.4$, and graphed the charge distributions for the numerical solution obtained.

The local velocities v_0^R and v_0^L are shown in figures 8 and 9, respectively. Here, trajectory 0 is at the base energy 2.4. The upper trajectory has been labelled -1; v_{-1}^R and v_{-1}^L are shown in figures 10 and 11.

Since the electron energy will in fact be distributed in some wavepacket around the

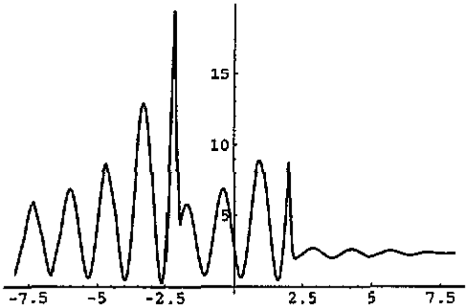

Figure 10. v^{R}_{-1} versus position.

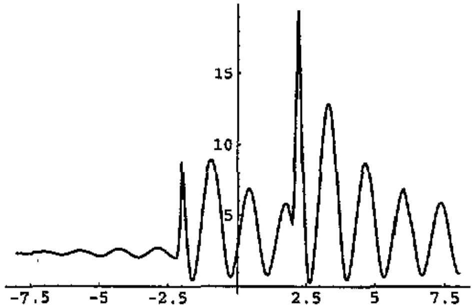

Figure 11. v^{L}_{-1} versus position.

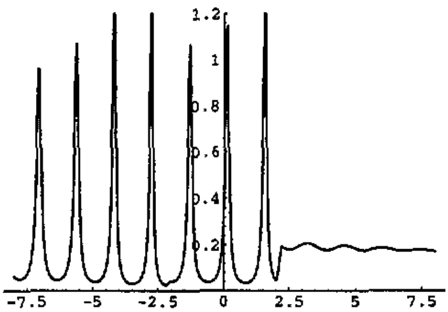

Figure 12. q^{R}_{0} versus position.

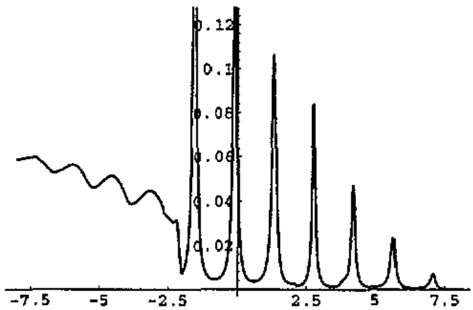

Figure 13. q^{L}_{0} versus position.

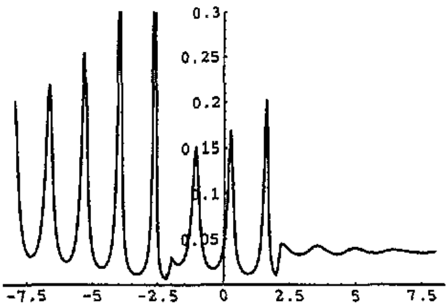

Figure 14. q^{R}_{-1} versus position.

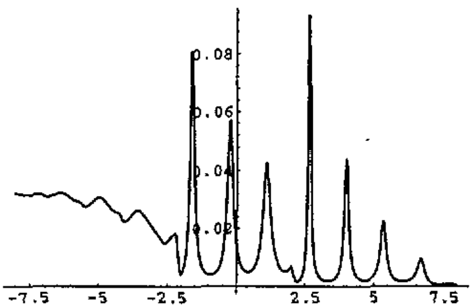

Figure 15. q^{L}_{-1} versus position.

energy of each trajectory, the technique would probably be improved by some form of smoothing (particularly outside the resonant region). For the present, unsmoothed results are used; we do not think this introduces too great an error with respect to total charge and transmission profiles.

Figures 12–15 show the individual charge distributions obtained. Figure 16 shows the charge density on trajectory 0, and figure 17 shows that of trajectory -1. The total charge density is shown in figure 18. Again, note that the spikes are probably artifacts of the approximation technique and would be strongly damped outside the central region by a more careful analysis.

The boundary conditions used to obtain these results are similar to those used in analysis of the Landauer formula. Electrons are assumed to enter the system as plane waves from a

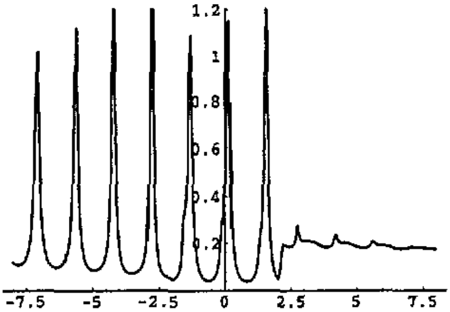

Figure 16. q_0 versus position.

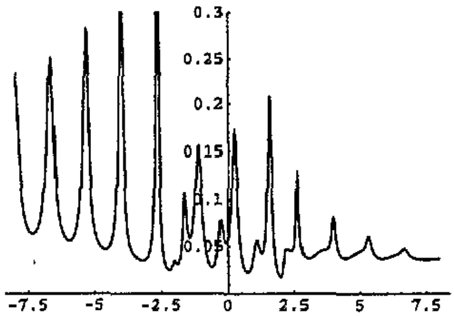

Figure 17. q_{-1} versus position.

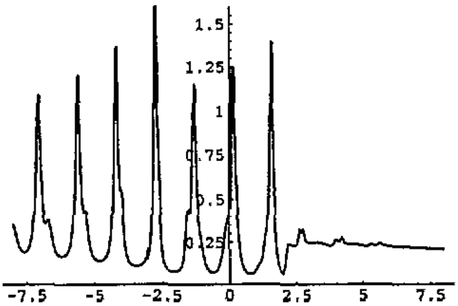

Figure 18. q versus position.

hypothetical reservoir to the left of the device. The reservoir is assumed to be in thermal equilibrium with the optical phonon bath.

Acknowledgment

We wish to thank Dr D C Herbert for a most stimulating discussion.

Appendix A. Details of the evaluation of the integral in (11)

$$\left[\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t)\,,\left[\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t'),\rho_{\mathrm{S}}^{\mathrm{I}}(t)\,\rho_{\mathrm{B}}^{\mathrm{I}}\right]\right]=\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t)\,\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t')\rho_{\mathrm{S}}^{\mathrm{I}}(t)\,\rho_{\mathrm{B}}^{\mathrm{I}}-\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t)\,\rho_{\mathrm{S}}^{\mathrm{I}}(t)\,\rho_{\mathrm{B}}^{\mathrm{I}}\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t')+\mathrm{HC}\,. \tag{A1}$$

Now on using (8) and (9)

$$\begin{aligned}
-\int_0^t \mathrm{Tr_B}\left(\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t)\,\mathcal{H}_{\mathrm{SB}}^{\mathrm{I}}(t')\rho_{\mathrm{S}}^{\mathrm{I}}(t)\,\rho_{\mathrm{B}}^{\mathrm{I}}\right)\mathrm{d}t'
&= -\int_0^t \mathrm{d}t'\,\mathrm{Tr_B}\,\gamma^2 \sum_{E_0E_1E_2E_3}\int \mathrm{d}x\,\mathrm{d}x'\,\mathrm{e}^{\mathrm{i}(E_0-E_1)t}\mathrm{e}^{\mathrm{i}(E_2-E_3)t'} \\
&\quad \times \mathcal{A}_{E_0}^{\dagger}\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}\mathcal{A}_{E_2}^{\dagger}\langle E_2|x'\rangle\langle x'|E_3\rangle\mathcal{A}_{E_3}\rho_{\mathrm{S}}^{\mathrm{I}}(t) \\
&\quad \times \sum_k\sum_{k'}\left(\mathrm{e}^{\mathrm{i}kx}C_k{}^{\mathrm{I}}(t)+\mathrm{e}^{-\mathrm{i}kx}C_k^{\dagger\,\mathrm{I}}(t)\right)\left(\mathrm{e}^{\mathrm{i}k'x'}C_{k'}{}^{\mathrm{I}}(t')+\mathrm{e}^{-\mathrm{i}k'x'}C_{k'}^{\dagger\,\mathrm{I}}(t')\right)\rho_{\mathrm{B}}
\end{aligned} \tag{A2a}$$

$$= -\int_0^t dt'\,\gamma^2 \sum_{E_0E_1E_2E_3} \int dx\,dx'\,e^{i(E_0-E_1)t} e^{i(E_2-E_3)t'}$$
$$\times \mathcal{A}^\dagger_{E_0}\langle E_0|x\rangle\langle x|E_1\rangle \mathcal{A}_{E_1}\mathcal{A}^\dagger_{E_2}\langle E_2|x'\rangle\langle x'|E_3\rangle\mathcal{A}_{E_3}\rho^{\mathrm{I}}_{\mathrm{S}}(t)$$
$$\times \sum_k \left\{ e^{ik(x-x')}e^{-\eta(t-t')}e^{-i\omega(t-t')}(\bar{n}+1) + e^{-ik(x-x')}e^{-\eta(t-t')}e^{i\omega(t-t')}\bar{n} \right\}. \tag{A2b}$$

It is assumed that $\eta t \gg 1$ and so

$$\int_0^t e^{-\eta(t-t')}\exp[itA + it'B]dt' \approx e^{i(A+B)t}\frac{1}{iB+\eta} \tag{A3a}$$
$$= \exp\left[i\,(A+B)\,t\right]\left(\pi\delta(B) - i\mathcal{P}\frac{1}{B}\right) \tag{A3b}$$

if we subsequently take the limit $\eta \longrightarrow 0^+$. Hence

$$-\int_0^t \mathrm{Tr}_{\mathrm{B}}\left(\mathcal{H}^{\mathrm{I}}_{\mathrm{SB}}(t)\,\mathcal{H}^{\mathrm{I}}_{\mathrm{SB}}(t')\rho^{\mathrm{I}}_{\mathrm{S}}(t)\,\rho^{\mathrm{I}}_{\mathrm{B}}\right)dt'$$
$$= -2\pi\gamma^2 \sum_{E_0E_1E_2E_3}\int dx\,e^{iE_0t}\mathcal{A}^\dagger_{E_0}\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}e^{-iE_1t}$$
$$\times e^{iE_2t}\mathcal{A}^\dagger_{E_2}\langle E_2|x\rangle\langle x|E_3\rangle\mathcal{A}_{E_3}e^{-iE_3t}\rho^{\mathrm{I}}_{\mathrm{S}}(t)$$
$$\times\left\{\bar{n}\left[\pi\delta(E_2-E_3-\omega) - \frac{i\mathcal{P}}{E_2-E_3-\omega}\right]\right.$$
$$\left. + (\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega) - \frac{i\mathcal{P}}{E_2-E_3+\omega}\right]\right\}. \tag{A4}$$

The contribution from the other term in (A1) is

$$\int_0^t \mathrm{Tr}_{\mathrm{B}}\left(\mathcal{H}^{\mathrm{I}}_{\mathrm{SB}}(t)\,\rho^{\mathrm{I}}_{\mathrm{S}}(t)\,\rho^{\mathrm{I}}_{\mathrm{B}}\mathcal{H}^{\mathrm{I}}_{\mathrm{SB}}(t')\right)dt' = \int_0^t dt'\,\mathrm{Tr}_{\mathrm{B}}\gamma^2\sum_{E_0E_1E_2E_3}\int dx\,dx'\,e^{i(E_0-E_1)t}e^{i(E_2-E_3)t'}$$
$$\times\mathcal{A}^\dagger_{E_0}\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}\rho^{\mathrm{I}}_{\mathrm{S}}(t)\,\mathcal{A}^\dagger_{E_2}\langle E_2|x'\rangle\langle x'|E_3\rangle\mathcal{A}_{E_3}$$
$$\times\sum_{k,k'}\left(e^{ikx}\mathcal{C}_k{}^{\mathrm{I}}(t) + e^{-ikx}\mathcal{C}^{\dagger\mathrm{I}}_k(t)\right)\rho^{\mathrm{I}}_{\mathrm{B}} big(e^{ik'x'}\mathcal{C}_{k'}{}^{\mathrm{I}}(t') + e^{-ik'x'}\mathcal{C}^{\dagger}_{k'}{}^{\mathrm{I}}(t')) \tag{A5a}$$
$$= \int_0^t dt'\,\gamma^2\sum_{E_0E_1E_2E_3}\int dx\,dx'\,e^{i(E_0-E_1)t}e^{i(E_2-E_3)t'}$$
$$\times\mathcal{A}^\dagger_{E_0}\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}\rho^{\mathrm{I}}_{\mathrm{S}}(t)\,\mathcal{A}^\dagger_{E_2}\langle E_2|x'\rangle\langle x'|E_3\rangle\mathcal{A}_{E_3}$$
$$\times\sum_k\left\{e^{ik(x-x')}e^{-\eta(t-t')}e^{-i\omega(t-t')}\bar{n} + e^{-ik(x-x')}e^{-\eta(t-t')}e^{i\omega(t-t')}(\bar{n}+1)\right\}$$
$$= 2\pi\gamma^2\sum_{E_0E_1E_2E_3}\int dx\,e^{iE_0t}\mathcal{A}^\dagger_{E_0}\langle E_0|x\rangle\langle x|E_1\rangle\mathcal{A}_{E_1}e^{-iE_1t}\rho^{\mathrm{I}}_{\mathrm{S}}(t)$$
$$\times e^{iE_2t}\mathcal{A}^\dagger_{E_2}\langle E_2|x\rangle\langle x|E_3\rangle\mathcal{A}_{E_3}e^{-iE_3t}$$
$$\times\left\{\bar{n}\left[\pi\delta(E_2-E_3+\omega) - \frac{i\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left. + (\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega) - \frac{i\mathcal{P}}{E_2-E_3-\omega}\right]\right\}. \tag{A5b}$$

This leads to (15). The one particle reduction of this master equation based on (19), (25), (21) and (22) gives

$$\frac{\mathrm{d}\rho^{(1)}}{\mathrm{d}t} = -\mathrm{i}\big[\mathcal{H}^{(1)}, \rho^{(1)}\big] + 2\pi\gamma^2 \sum_{E_0 E_1 E_2 E_3} \int \mathrm{d}x\, |E_1\rangle\, \langle E_2|x\rangle\langle x|E_3\rangle\, \langle E_0|\, \mathrm{Tr}\, \mathcal{A}^\dagger_{E_0}\mathcal{A}_{E_1}$$
$$\times\Bigg\{\big[\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\rho_\mathrm{S}\mathcal{A}^\dagger_x\mathcal{A}_x - \mathcal{A}^\dagger_x\mathcal{A}_x\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\rho_\mathrm{S}\big]$$
$$\times\Bigg[(\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]$$
$$+\bar{n}\left[\pi\delta(E_2-E_3-\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\Bigg]$$
$$+\left[\mathcal{A}^\dagger_x\mathcal{A}_x\rho_\mathrm{S}\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3} - \rho_\mathrm{S}\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\mathcal{A}^\dagger_x\mathcal{A}_x\right]$$
$$\times\Bigg[\bar{n}\left[\pi\delta(E_2-E_3+\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]$$
$$+(\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\Bigg]\Bigg\} \qquad \text{(A6}a\text{)}$$

$$= -\mathrm{i}\big[\mathcal{H}^{(1)}, \rho^{(1)}\big] + 2\pi\gamma^2 \sum_{E_0 E_1 E_2 E_3} \int \mathrm{d}x\, |E_1\rangle\, \langle E_2|x\rangle\langle x|E_3\rangle\, \langle E_0|\, \mathrm{Tr}\, \rho_\mathrm{S}$$
$$\times\Bigg\{\big[\mathcal{A}^\dagger_x\mathcal{A}_x\mathcal{A}^\dagger_{E_0}\mathcal{A}_{E_1}\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3} - \mathcal{A}^\dagger_{E_0}\mathcal{A}_{E_1}\mathcal{A}^\dagger_x\mathcal{A}_x\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\big]$$
$$\times\Bigg[(\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]$$
$$+\bar{n}\left[\pi\delta(E_2-E_3-\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\Bigg]$$
$$+\big[\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\mathcal{A}^\dagger_{E_0}\mathcal{A}_{E_1}\mathcal{A}^\dagger_x\mathcal{A}_x - \mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\mathcal{A}^\dagger_x\mathcal{A}_x\mathcal{A}^\dagger_{E_0}\mathcal{A}_{E_1}\big]$$
$$\times\Bigg[\bar{n}\left[\pi\delta(E_2-E_3+\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]$$
$$+(\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\Bigg]\Bigg\} \qquad \text{(A6}b\text{)}$$

$$= -\mathrm{i}\big[\mathcal{H}^{(1)}, \rho^{(1)}\big] + 2\pi\gamma^2 \sum_{E_0 E_1 E_2 E_3} \int \mathrm{d}x\, |E_1\rangle\, \langle E_2|x\rangle\langle x|E_3\rangle\, \langle E_0|\, \mathrm{Tr}\, \rho_\mathrm{S}$$
$$\times\Bigg\{\big[\mathcal{A}^\dagger_x\mathcal{A}_{E_1}\langle x|E_0\rangle - \mathcal{A}^\dagger_{E_0}\mathcal{A}_x\langle E_1|x\rangle\big]\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}$$
$$\times\Bigg[(\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]$$
$$+\bar{n}\left[\pi\delta(E_2-E_3-\omega) - \frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\Bigg]$$
$$+\mathcal{A}^\dagger_{E_2}\mathcal{A}_{E_3}\big[\mathcal{A}^\dagger_{E_0}\mathcal{A}_x\langle E_1|x\rangle - \mathcal{A}^\dagger_x\mathcal{A}_{E_1}\langle x|E_0\rangle\big]$$

$$\times\left[\bar{n}\left[\pi\delta(E_2-E_3+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left.\left.+(\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\right]\right\} \tag{A6c}$$

$$= -\mathrm{i}\left[\mathcal{H}^{(1)},\rho^{(1)}\right]+2\pi\gamma^2\sum_{E_0E_1E_2E_3}\int \mathrm{d}x\,|E_1\rangle\,\langle E_2|x\rangle\langle x|E_3\rangle\,\langle E_0|$$
$$\times\left\{\left[\langle E_3|\,\rho^{(1)}\,|x\rangle\,\langle E_1|E_2\rangle\langle x|E_0\rangle-\langle E_3|\,\rho^{(1)}\,|E_0\rangle\,\langle x|E_2\rangle\langle E_1|x\rangle\right]\right.$$
$$\times\left[(\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left.+\bar{n}\left[\pi\delta(E_2-E_3-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\right]$$
$$+\left[\mathrm{Tr}\big(\rho_{\mathrm{S}}\mathcal{A}^{\dagger}_{E_0}\mathcal{A}^{\dagger}_{E_2}\mathcal{A}_x\mathcal{A}_{E_3}\big)\langle E_1|x\rangle-\mathrm{Tr}\big(\rho_{\mathrm{S}}\mathcal{A}^{\dagger}_x\mathcal{A}^{\dagger}_{E_2}\mathcal{A}_{E_1}\mathcal{A}_{E_3}\big)\langle x|E_0\rangle\right]$$
$$\times\left[(\bar{n}+1)\left[\pi\delta(E_2-E_3+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left.+\bar{n}\left[\pi\delta(E_2-E_3-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\right]$$
$$+\left[\langle x|\,\rho^{(1)}\,|E_2\rangle\,\langle E_3|E_0\rangle\langle E_1|x\rangle-\langle E_1|\,\rho^{(1)}\,|E_2\rangle\,\langle E_3|x\rangle\langle x|E_0\rangle\right]$$
$$\times\left[\bar{n}\left[\pi\delta(E_2-E_3+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left.+(\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\right]$$
$$+\left[\mathrm{Tr}\big(\rho_{\mathrm{S}}\mathcal{A}^{\dagger}_{E_2}\mathcal{A}^{\dagger}_x\mathcal{A}_{E_3}\mathcal{A}_{E_1}\big)\langle x|E_0\rangle-\mathrm{Tr}\big(\rho_{\mathrm{S}}\mathcal{A}^{\dagger}_{E_2}\mathcal{A}^{\dagger}_{E_0}\mathcal{A}_{E_3}\mathcal{A}_x\big)\langle E_1|x\rangle\right]$$
$$\times\left[\bar{n}\left[\pi\delta(E_2-E_3+\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3+\omega}\right]\right.$$
$$\left.\left.+(\bar{n}+1)\left[\pi\delta(E_2-E_3-\omega)-\frac{\mathrm{i}\mathcal{P}}{E_2-E_3-\omega}\right]\right]\right\}. \tag{A6d}$$

Appendix B.

$$-\int_0^t \mathrm{Tr}_{\mathrm{B}'}\mathcal{H}^{\mathrm{I}}_{\mathrm{S'B'}}(t)\,\mathcal{H}^{\mathrm{I}}_{\mathrm{S'B'}}(t')\rho^{\mathrm{I}}_{\mathrm{S'}}(t)\,\rho^{\mathrm{I}}_{\mathrm{B'}}\,\mathrm{d}t'$$
$$= -\int_0^t \mathrm{d}t'\mathrm{Tr}_{\mathrm{B}'}\gamma^2\sum_{tr}\sum_{tr'}\sum_{E\sigma}\sum_{E'\sigma'}\sum_{E''\sigma''}\sum_{E'''\sigma'''}\sum_{k}\int \mathrm{d}x\,\mathrm{d}x' \tag{B1a}$$
$$\times\Big\{\,|E\sigma,tr-1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\,\big\langle E'\sigma',tr\big|\,\mathrm{e}^{\mathrm{i}(E-E'-\omega)t}$$
$$\times\big|E''\sigma'',tr'\big\rangle\langle E''\sigma''|x'\rangle\langle x'|E'''\sigma'''\rangle\big\langle E'''\sigma''',tr'-1\big|$$
$$\times\mathrm{e}^{\mathrm{i}(E''-E'''+\omega)t'}\rho^{\mathrm{I}}_{\mathrm{S'}}(t)\,\mathrm{e}^{\mathrm{i}k(x-x')}\mathrm{e}^{-\eta(t-t')}\,(\bar{n}+1)$$
$$+|E\sigma,tr\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\,\big\langle E'\sigma',tr-1\big|\,\mathrm{e}^{\mathrm{i}(E-E'+\omega)t}$$
$$\times\big|E''\sigma'',tr'-1\big\rangle\langle E''\sigma''|x'\rangle\langle x'|E'''\sigma'''\rangle\big\langle E'''\sigma''',tr'\big|$$
$$\times\mathrm{e}^{\mathrm{i}(E''-E'''-\omega)t'}\rho^{\mathrm{I}}_{\mathrm{S'}}(t)\,\mathrm{e}^{-\mathrm{i}k(x-x')}\mathrm{e}^{-\eta(t-t')}\bar{n}\Big\} \tag{B1b}$$

$$
\begin{aligned}
&= -2\pi\gamma^2 \sum_{tr}\sum_{E\sigma}\sum_{E'\sigma'}\sum_{E'''\sigma'''}\int \mathrm{d}x \\
&\times\Big\{ e^{\mathrm{i}Et}\,|E\sigma, tr-1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle \\
&\times\langle E'\sigma'|x\rangle\langle x|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr-1\big|\, e^{-\mathrm{i}E'''t}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\times(\bar{n}+1)\left[\pi\delta\big(E'-E'''+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E'-E'''+\omega}\right] \\
&+e^{\mathrm{i}Et}\,|E\sigma, tr\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle \\
&\times\langle E'\sigma'|x\rangle\langle x|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr\big|\, e^{-\mathrm{i}E'''t}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\times\bar{n}\left[\pi\delta\big(E'-E'''+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E'-E'''+\omega}\right]\Big\}
\end{aligned}
\tag{B1c}
$$

$$
\begin{aligned}
&= -2\pi\gamma^2 \sum_{tr}\sum_{E\sigma}\sum_{E'\sigma'}\sum_{E'''\sigma'''}\int \mathrm{d}x \\
&\times e^{\mathrm{i}Et}\,|E\sigma, tr\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle \\
&\times\langle E'\sigma'|x\rangle\langle x|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr\big|\, e^{-\mathrm{i}E'''t}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\times\Big\{(\bar{n}+1)\left[\pi\delta\big(E'-E'''+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E'-E'''+\omega}\right] \\
&+\bar{n}\left[\pi\delta\big(E'-E'''+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E'-E'''+\omega}\right]\Big\}.
\end{aligned}
\tag{B1d}
$$

Also

$$
\begin{aligned}
&\int_0^t \mathrm{Tr}_{\mathrm{B}'}\mathcal{H}^{\mathrm{I}}_{\mathrm{S'B'}}(t)\,\rho^{\mathrm{I}}_{\mathrm{S}'}(t)\,\rho^{\mathrm{I}}_{\mathrm{B}'}\mathcal{H}^{\mathrm{I}}_{\mathrm{S'B'}}(t')\,\mathrm{d}t' \\
&\quad= \int_0^t \mathrm{d}t'\mathrm{Tr}_{\mathrm{B}'}\gamma^2 \sum_{tr}\sum_{tr'}\sum_{E\sigma}\sum_{E'\sigma'}\sum_{E''\sigma''}\sum_{E'''\sigma'''}\sum_{k}\int \mathrm{d}x\,\mathrm{d}x' \\
&\quad\times\Big\{\,|E\sigma, tr-1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\big\langle E'\sigma', tr\big|\, e^{\mathrm{i}(E-E'-\omega)t}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\quad\times\big|E''\sigma'', tr\big\rangle\langle E''\sigma''|x'\rangle\langle x'|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr-1\big|\, e^{\mathrm{i}(E''-E'''+\omega)t'} \\
&\quad\times e^{\mathrm{i}k(x-x')}e^{-\eta(t-t')}\bar{n} \\
&\quad+|E\sigma, tr+1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\big\langle E'\sigma', tr\big|\, e^{\mathrm{i}(E-E'-\omega)t}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\quad\big|E''\sigma'', tr\big\rangle\langle E''\sigma''|x'\rangle\langle x'|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr+1\big|\, e^{\mathrm{i}(E''-E'''+\omega)t'} \\
&\quad e^{-\mathrm{i}k(x-x')}e^{-\eta(t-t')}e^{\mathrm{i}\omega(t-t')}\,(\bar{n}+1)\Big\}
\end{aligned}
\tag{B2a}
$$

$$
\begin{aligned}
&= 2\pi\gamma^2 \sum_{tr}\sum_{E\sigma}\sum_{E'\sigma'}\sum_{E''\sigma''}\sum_{E'''\sigma'''}\int \mathrm{d}x \\
&\times\Big\{ e^{\mathrm{i}Et}\,|E\sigma, tr-1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\big\langle E'\sigma', tr\big|\, e^{-\mathrm{i}E't}\rho^{\mathrm{I}}_{\mathrm{S}'}(t) \\
&\times e^{\mathrm{i}E''t}\big|E''\sigma'', tr\big\rangle\langle E''\sigma''|x\rangle\langle x|E'''\sigma'''\rangle\big\langle E'''\sigma''', tr-1\big|\, e^{-\mathrm{i}E'''t} \\
&\bar{n}\left[\pi\delta\big(E''-E'''+\omega\big)-\frac{\mathrm{i}\mathcal{P}}{E''-E'''+\omega}\right] \\
&+e^{\mathrm{i}Et}\,|E\sigma, tr+1\rangle\,\langle E\sigma|x\rangle\langle x|E'\sigma'\rangle\big\langle E'\sigma', tr\big|\, e^{-\mathrm{i}E't}\rho^{\mathrm{I}}_{\mathrm{S}'}(t)
\end{aligned}
$$

$$\times e^{iE''t} \left|E''\sigma'', tr\right\rangle \langle E''\sigma''|x\rangle\langle x|E'''\sigma'''\rangle \left\langle E'''\sigma''', tr+1\right| e^{-iE'''t}$$

$$\times (\bar{n}+1) \left[\pi\delta\left(E''-E'''-\omega\right) - \frac{i\mathcal{P}}{E''-E'''-\omega}\right]\Bigg\} . \qquad \text{(B2}b\text{)}$$

References

[1] Ferry D K and Grondin R O 1991 *Physics of Submicron Devices* (New York: Plenum)

[2] Herbert D C 1984 *J. Phys. C: Solid State Phys.* **17** 6749.

[3] Till S J and Herbert D C 1983 *J. Phys. C: Solid State Phys.* **16** 5849

[4] Herbert D C, Jefferson J H and Anderson J D 1989 A new approach to modelling microstructures and sub-micron devices *Proc. Nasecode VI*

[5] Herbert D C 1991 *Semicond. Sci. Technol.* **6** 405

[6] Fetter A L and Walecka J D 1971 *Quantum Theory of Many-Particle Systems* (New York: McGraw-Hill)

[7] Pike E R and Sarkar S 1995 *The Quantum Theory of Radiation* (Oxford: Oxford University) to be published

[8] Louisell W H 1973 *Quantum Statistical Properties of Radiation* (New York: Wiley)

[9] Herbert D C, Jefferson J H and Kirton M J 1985 *Physica* **134B** 82

[10] Wolfram S 1991 *Mathematica—A System for Doing Mathematics by Computer* 2nd edn (Redwood City, CA: Addison-Wesley)