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A Master Equation Approach to the Simulation of Electron Transport in Small Semiconductor Devices

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1. Introduction

In a semiconductor device of size L smaller than the electron dephasing length in the contacts, $\lambda_\phi \approx \hbar v_{th}/\delta E_{th}$, where v_{th} and δE_{th} are the thermal velocity and energetic broadening, electrons are injected as packets 'larger' than the device itself. In terms of the density-matrix ρ , this means that the contacts inject only diagonal elements of ρ , in the representation of the eigenstates of the device. Van Hove[1] has observed that, starting from a quasi-diagonal density matrix (that is, with off-diagonal elements nonvanishing only when mixing states within a small energy range, $\sim \delta E_{th}$ in our case), the time needed to build the off-diagonal elements of the density matrix ρ is of the order of $\hbar/\delta E_{th}$. This time-scale, $\hbar/\delta E_{th}$, is much longer than both the hot-electron relaxation time and the transit time, L/v , where v is the hot-electron drift velocity. Thus, the build-up of off-diagonal terms of ρ occurs only long after the electron has gone through the device and relaxed in the collector reservoir. It follows that a simple master equation which takes into account only the diagonal elements of the density matrix is sufficient to describe electron transport in these small devices.

These ideas have been presented before[2]. The purpose of this paper is to sketch a 'formal' derivation of the transport equation, emphasizing the crucial approximations required, and to extend the method to more realistic band structures. The example of electron transport in an *nin* diode is finally presented.

2. The Transport Equation

Closed systems, single particle

Let's consider a semiconductor in thermal contact with a heat bath. The Hamiltonian of the system is $H = H_{el} + H_{ph} + H_{ep}$, where $H_{el} = \mathcal{T} - eV(\mathbf{r})$ is the single-electron Hamiltonian, $V(\mathbf{r})$ is the Hartree potential and \mathcal{T} is the kinetic-energy operator. The eigenstates and eigenvalues of H_{el} are denoted by $|\mu\rangle$ and E_μ , respectively. Omitting phonon-branch indices, the phonon Hamiltonian H_{ph} is $\sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$ where $a_{\mathbf{q}}$ ($a_{\mathbf{q}}^\dagger$) is the annihilation (creation) operator of a phonon of

wavevector \mathbf{q} and energy $\hbar\omega_{\mathbf{q}}$. In the representation of the eigenstates $\{|\mu\rangle\}$, the electron-phonon Hamiltonian is $H_{ep} \equiv \alpha H' = i\alpha \sum_{\mathbf{q}\mu\nu} [\mathcal{F}_{\mathbf{q}\mu\nu} a_{\mathbf{q}} - \mathcal{F}_{\mathbf{q}\mu\nu}^* a_{\mathbf{q}}^\dagger]$, where $\mathcal{F}_{\mathbf{q}\mu\nu} = (1/\alpha) \langle \mu | F_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r}) | \nu \rangle$ is the electron-phonon matrix element, and α is the dimensionless interaction coupling constant.

The equation of motion for the density-matrix ρ is the Liouville-von Neumann equation. In the Heisenberg representation this can be written as:

$$\begin{aligned} \frac{\partial \rho(t)}{\partial t} = & -\frac{i}{\hbar} [H_0(t), \rho(t)] - \frac{i}{\hbar} \alpha [H'(t), \rho(0)] \\ & - \frac{\alpha}{\hbar^2} \int_0^t dt' [H'(t), [H_0(t'), \rho(t')]] \\ & - \frac{\alpha^2}{\hbar^2} \int_0^t dt' [H'(t), [H'(t'), \rho(t')]], \end{aligned} \quad (1)$$

where $H_0 = H_{el} + H_{ph}$. In the weak-coupling limit ($\alpha^2 \ll 1$) and considering the time evolution to the leading order in α - that is, up to times of the order of the Van Hove time $t \sim O(\alpha^{-2})$, coupled electron-phonon modes may be ignored and the full density-matrix may be factored into the product of the normalized electron and the phonon density matrices as $\rho(t) \approx \rho^{(ph)}(t) \otimes \rho^{(el)}(t)$ where $\rho^{(ph)}(t) = \sum_{\{n_{\mathbf{q}}\}} \rho_{\{n_{\mathbf{q}}\}}^{(ph)}(t) |\{n_{\mathbf{q}}\}\rangle \langle \{n_{\mathbf{q}}\}|$ is assumed diagonal in the occupation-number representation $\{n_{\mathbf{q}}\}$, and $\rho^{(el)}(t) = \sum_{\mu\nu} c_\mu(t) c_\nu^*(t) |\mu\rangle \langle \nu|$.

We are now interested in the reduced electronic density matrix $\rho^{(el)}(t) = Tr_{ph}[\rho(t)]$, where Tr_{ph} is the trace over the 'irrelevant'[3] phonon degrees of freedom. Since terms of odd order in α involve an odd number of H' factors, they vanish upon tracing over bath states. Thus, the equation of motion for the matrix elements $\rho_{\mu\mu'}^{(el)} = \langle \mu | Tr_{ph} \rho | \mu' \rangle = c_\mu c_{\mu'}^*$ of the reduced (electronic) density operator can be written as:

$$\begin{aligned} \frac{\partial \rho_{\mu\mu'}^{(el)}(t)}{\partial t} = & -\frac{i}{\hbar} (E_\mu - E_{\mu'}) \rho_{\mu\mu'}^{(el)}(t) - \\ & \frac{\alpha^2}{\hbar^2} \int_0^t dt' \sum_{\{n_{\mathbf{q}}\}} \langle \{n_{\mathbf{q}}\} \mu | [H'(t), [H'(t'), \rho(t')]] | \{n_{\mathbf{q}}\} \mu' \rangle \end{aligned} \quad (2)$$

The last term on the right-hand-side of Eq. (2) can be decomposed into out- and in-scattering terms. The integrand of the first out-scattering term can be written as:

$$-\frac{\alpha^2}{\hbar^2} \sum_{\{n_{\mathbf{q}}\}\{n'_{\mathbf{q}}\}} \sum_{\nu\lambda} \rho_{\{n_{\mathbf{q}}\}}^{(ph)}(t') c_{\nu}(t') c_{\mu'}^*(t') \\ \times \langle \{n_{\mathbf{q}}\}\mu | H'(t) | \{n'_{\mathbf{q}}\}\lambda \rangle \langle \{n'_{\mathbf{q}}\}\lambda | H'(t') | \{n_{\mathbf{q}}\}\nu \rangle. \quad (3)$$

This term is of the Van Hove form[1]: For $\mu \neq \nu$, the sums over the bath degrees of freedom involve random phases, so that the overall contribution of these off-diagonal terms is of the order of N_b , the number of degrees of freedom of the heat bath. On the contrary, if $\mu = \nu$, the sums give an in-phase, coherent contribution of order N_b^2 . In the limit of infinitely large N_b , only terms for which $\mu = \nu$ survive. Thanks to this observation, to the leading order in α this term simplifies to:

$$-\frac{\alpha^2}{\hbar^2} \sum_{\mathbf{q}\lambda} |\mathcal{F}_{\mathbf{q}\mu\lambda}|^2 \langle n_{\mathbf{q}}(t') \rangle c_{\mu}(t') c_{\mu'}^*(t') \times \\ e^{-i(E_{\lambda} - E_{\mu} - \hbar\omega_{\mathbf{q}})(t-t')/\hbar} \equiv -\frac{1}{2} \sum_{\lambda} K_{\lambda\mu}^{(ab)}(t, t') \rho_{\mu\mu'}(t'), \quad (4)$$

having considered only absorption processes and having defined the average phonon number $\langle n_{\mathbf{q}}(t) \rangle = \sum_{\{n_{\mathbf{q}}\}} \rho_{\{n_{\mathbf{q}}\}}(t) \langle \{n_{\mathbf{q}}\} | a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} | \{n_{\mathbf{q}}\} \rangle$. Emission processes are characterized by a similar kernel. The second out-scattering term gives a similar contribution, with the electron state μ replaced by μ' . Therefore, the 'out-scattering' terms of the equation of motion can be written as:

$$\left(\frac{\partial \rho_{\mu\mu'}^{(el)}(t)}{\partial t} \right)_{out} = \\ - \sum_{\lambda} \int_0^t dt' \frac{1}{2} [K_{\lambda\mu}(t, t') + K_{\lambda\mu'}(t, t')] \rho_{\mu\mu'}^{(el)}(t'), \quad (5)$$

with $K_{\lambda\mu}(t, t') = K_{\lambda\mu}^{(ab)}(t, t') + K_{\lambda\mu}^{(em)}(t, t')$.

In-scattering terms in general contribute also to the off-diagonal elements (i.e., $\mu \neq \mu'$). However, as discussed above, Van Hove[1] has shown that starting from a quasi-diagonal density matrix (i.e., $c_{\mu}(0)c_{\mu'}^*(0) = 0$ for $E_{\mu} - E_{\mu'} > \delta E_{th} \ll \delta E_D$) and in the weak-coupling limit, off-diagonal elements are negligible up to times of the order of $t \sim O(\alpha^{-2})$. Indeed, for small α we can think of finding a solution of Eq. (2) by expanding it in powers of α . The leading order approximation (α^2) is obtained by replacing $\rho(t')$ with $\rho(0)$ in the last term of Eq. (2). Therefore, assuming that $\rho^{(el)}(0)$ is diagonal, the integrand associated with the first in-scattering term right-hand-side of Eq. (2) is also of the Van Hove form, up to terms of higher order in α , so that we can write its contribution as $(1/2) \sum_{\nu} K_{\mu\nu}(t, t') \rho_{\nu\nu}(t') \delta_{\mu\mu'}$. Since the second in-scattering term gives an identical contribution, the Liouville-von Neumann equation in the weak-coupling limit and for a diagonal initial electronic density matrix takes the form of Zwanzig's 'pre-master' equation[4,5]:

$$\frac{\partial \rho_{\mu\mu'}^{(el)}(t)}{\partial t} = -\frac{i}{\hbar} (E_{\mu} - E_{\mu'}) \rho_{\mu\mu'}^{(el)}(t)$$

$$- \sum_{\lambda} \int_0^t dt' \frac{1}{2} [K_{\lambda\mu}(t, t') + K_{\lambda\mu'}(t, t')] \rho_{\mu\mu'}^{(el)}(t') \\ + \sum_{\lambda} \int_0^t dt' \delta_{\mu\mu'} K_{\mu\lambda}(t, t') \rho_{\lambda\lambda}^{(el)}(t'). \quad (6)$$

Invoking now the Markov approximation, letting $\rho^{(ph)}(t) \equiv \rho^{(ph)}(0)$ at all times, and so assuming that the phonons remain at thermal equilibrium, $K_{\mu\nu}(t, t')$ becomes a functions of $t - t'$. However, this does not yet result in a loss of memory effects, since Eq. (6) is still reversible[5]. The essential step required to obtain the irreversible master equation is to consider the van Hove limit $\alpha^2 t \rightarrow \text{constant}$ as $\alpha^2 \rightarrow 0$ while $t \rightarrow \infty$. As described by Jancel, taking this limit and defining the 'Golden-rule' absorption rate $W_{\mu\lambda}^{(ab)} = (2\pi/\hbar)\alpha^2 \sum_{\mathbf{q}} |\mathcal{F}_{\mathbf{q}\mu\lambda}|^2 \times \langle n_{\mathbf{q}} \rangle \delta(E_{\mu} - E_{\lambda} - \hbar\omega_{\mathbf{q}})$ and similarly for $W_{\mu\lambda}^{(em)}$, we finally reach the master equation:

$$\frac{\partial \rho_{\mu\mu'}^{(el)}(t)}{\partial t} = -\frac{i}{\hbar} (E_{\mu} - E_{\mu'}) \rho_{\mu\mu'}^{(el)}(t) \\ - \sum_{\lambda} \frac{1}{2} [W_{\lambda\mu} + W_{\lambda\mu'}] \rho_{\mu\mu'}^{(el)}(t) + \sum_{\lambda} \delta_{\mu\mu'} W_{\mu\lambda} \rho_{\lambda\lambda}^{(el)}(t), \quad (7)$$

having set $W_{\lambda\mu} = W_{\lambda\mu}^{(ab)} + W_{\lambda\mu}^{(em)}$.

The price paid in taking the Van Hove limit is our inability to study the dynamics of the electron-phonon interaction at very short times[6-8]: At finite times, the real part of the kernel $K_{\lambda\mu}(t, t')$ is non positive-definite, due to the presence of a superposition of off-shell states, so that Eq. (5) reflects also the growth of the off-diagonal terms $\rho_{\mu\mu'}(t)$. Taking the van Hove limit amounts to assuming 'completed' collisions, resulting in a positive-definite scattering kernel and in the absence of the fast coming-and-going of these off-diagonal terms. As a consequence, to the leading order in α , the off-diagonal matrix elements $\rho_{\mu\nu}^{(el)}(t)$ decay exponentially in time at a rate $\sum_{\lambda} (W_{\lambda\mu} + W_{\lambda\nu})/2$, and remain negligibly small if $\rho^{(el)}(0)$ is quasi-diagonal. The equation for the diagonal terms is the 'usual' master equation:

$$\frac{\partial \rho_{\mu\mu}^{(el)}(t)}{\partial t} = \sum_{\lambda} [W_{\mu\lambda} \rho_{\lambda\lambda}^{(el)}(t) - W_{\lambda\mu} \rho_{\mu\mu}^{(el)}(t)]. \quad (8)$$

Closed systems, many particles

In order to account for the effects of statistics in a many-electron system, one has to consider the matrix elements of the reduced single-electron density operator, $\rho_{\mu\mu'}^{(el)}(t) = \langle c_{\mu}^{\dagger} c_{\mu'} \rangle_t$, c_{μ}^{\dagger} and c_{μ} now being the creation and annihilation operators for the single-electron states $|\mu\rangle$. In analogy with the procedure followed above, and making use of the same approximations, one obtains an equation involving as unknowns not only the one-particle density matrix elements $\langle c_{\mu}^{\dagger} c_{\mu'} \rangle_t$, but also the two-particle density matrix elements, $\langle c_{\lambda}^{\dagger} c_{\lambda} c_{\mu}^{\dagger} c_{\mu} \rangle_{\nu}$. These can be eliminated by invoking the Hartree-Fock approximation[9,10], so that $\langle c_{\mu}^{\dagger} c_{\nu} c_{\lambda} c_{\lambda}^{\dagger} \rangle_{\nu} \approx \langle c_{\mu}^{\dagger} c_{\nu} \rangle_{\nu}$

($1 - \langle c_\lambda^\dagger c_\lambda \rangle$). Using again the Van Hove limit and the Markov approximation, we recover the single-electron master equation, Eq. (8), corrected by the well-known Pauli exclusion terms.

Open systems

The open nature of the system has been recently handled by invoking the boundary conditions for the Wigner function, as so assuming the injection of pure plane waves[11]. Here the smallness of the device leads to the assumption that electrons are injected as completely delocalized objects into the scattering eigenstates. The electron source is assumed to be a quasi-equilibrium distribution $f^{(s)}(\mathbf{k}_s)$, where \mathbf{k}_s is the wavevector of the state injected from contact number s , such that $E(\mathbf{k}_s) = E_\mu - eV_s$, V_s being the electrostatic potential at the s -th contact. Thus, the master equation, Eq. (8), is augmented by an injection/extraction term:

$$\left(\frac{\partial \rho_\mu^{(s)}}{\partial t} \right)_{res} = |A_\mu^{(s)}|^2 v_\perp(\mathbf{k}_s) [f^{(s)}(\mathbf{k}_s + \mathbf{k}_d^{(s)}) - \rho_\mu^{(s)}], \quad (9)$$

where we have indicated with $\rho_\mu^{(s)}$ the diagonal matrix elements $\rho_{\mu s; \mu s}^{(el)}$ of the reduced single-electron density matrix taken over electron states $|\mu, s\rangle$ associated with the injection from the s -th contact. $A_\mu^{(s)}$ is a suitable – as discussed below – normalization of the wavefunction $\zeta_\mu^{(s)}(\mathbf{r})$, satisfying the required (open) boundary conditions, and $v_\perp(\mathbf{k}_s)$ is the component of the group velocity normal to the device/ s -contact boundary. Finally, the shift $\mathbf{k}_d^{(s)}$ in momentum space is required to ensure charge neutrality near the contacts and/or conservation of flux across the device-contact boundaries. Several schemes have been proposed to determine $\mathbf{k}_d^{(s)}$ [2,12,13]. Here it is determined self-consistently to ensure current continuity across the device-contacts boundaries.

3. Band Structure Effects

Within the envelope (or effective mass) approximation and ignoring interband effects, as appropriate for electrons in Si at moderate electric fields, the kinetic energy operator \mathcal{T} is approximated by the operator $E(-i\nabla)$, where $E(\mathbf{k})$ is the electron dispersion in the lowest-lying conduction band. Considering a one dimensional problem, $V(\mathbf{r}) = V(z)$, and indicating with κ the transverse component of the electron wavevector \mathbf{k} , for each κ the ‘envelope’ $\zeta_\kappa(z)$ satisfies the Wannier equation:

$$\left[E\left(\kappa, -i\frac{d}{dz}\right) + eV(z) \right] \zeta_\kappa(z) = E \zeta_\kappa(z). \quad (10)$$

One way to solve Eq. (10) is to employ Fourier transforms. This, however, does not yield the left- and right-traveling scattering states, which must be obtained following an alternate approach in real space. A possible real-space approach consists in using the interpolation scheme employed in Ref. [14], which leads to the piece-wise cubic interpolation $E_\kappa(k_z) = \sum_{n=0}^N \Lambda_\kappa^{(n)}(E) |k_z|^n$ with $N = 3$,

as so to a third-order differential equation of the form:

$$i\Lambda_\kappa^{(3)} \frac{d^3 \zeta_\kappa(z)}{dz^3} - \Lambda_\kappa^{(2)} \frac{d^2 \zeta_\kappa(z)}{dz^2} - i\Lambda_\kappa^{(1)} \frac{d \zeta_\kappa(z)}{dz} + [\Lambda_\kappa^{(0)} + eV(z)] \zeta_\kappa(z) = E_\kappa \zeta_\kappa(z), \quad (11)$$

where the coefficients $\Lambda_\kappa^{(n)}$ are piecewise-constant functions of $E_\kappa - eV(z)$. The symmetrization of the dispersion around the band minima, always possible by the symmetry of the crystal and the nature of the Bloch expansion, ensures the hermiticity of the problem.

A major problem affecting all nonparabolic formulations of the form above with $N > 2$, is the presence of spurious (unphysical) solutions, as the interpolation is only valid locally in k -space. Therefore, care must be taken to ensure that spurious solutions will not propagate and that, in addition to the physical solution k_{phys} of the algebraic cubic equation associated with Eq. (11), the other root will be $-k_{phys}$, or $G_z - k_{phys}$, where \mathbf{G} is a wavevector of the reciprocal lattice, and the transmission and reflection coefficients for scattering states will satisfy the unitarity relationship. Whenever in a given mesh element in k -space the coefficients $\Lambda_\kappa^{(n)}$ do not guarantee this, the interpolation is collapsed to a local parabola.

The current density associated with the solutions of Eq. (11) can be obtained from Green’s identity, where the ‘prime’ stands for d/dz . The Hermiticity condition ensures that $\partial j_\kappa(z)/\partial z = 0$ for stationary states. In particular, the constant current density (or probability flux) associated with a plane wave is $j_\kappa(z) = v_z(\kappa, k_z) |\zeta_\kappa(z)|^2$, as expected.

Finally, the density of states, the Fermi functions, and the nonpolar electron-phonon scattering rates are computed in analogy to what done in the bulk[14]. For a device homogeneous in the (x, y) -plane, the (k_x, k_y) -plane is discretized into ‘squares’ of side $\Delta\kappa$. The density of states in each square is obtained following a simplification of the Gilat-Raubenheimer algorithm[15].

4. An example

In this section we consider the *nin* Si diode already described in Ref. [2], but now using the more realistic Si band structure and scattering processes employed in the bulk model of Ref. [14]. The space of transverse \mathbf{k} -vectors κ , is discretized into squares of side $\Delta\kappa = 0.05(2\pi/a)$, while the dispersion along the direction of motion, $E(\kappa, k_z)$, is known over a one-dimensional mesh of 41 k_z -points in the interval $[-1, +1] (2\pi/a)$. Starting from a first ‘guess’ for the potential $V(z)$, for each κ , Eq. (10) is first solved by Fourier-transforms over sines and cosines. These ‘standing’ electron states are then normalized to $\int_0^L dz |\zeta_{\mu\kappa}(z)|^2 = 1/2$. Having so determined the eigenvalues $E_{\mu\kappa}$, only states of low-enough energy ($E_{\mu\kappa} \leq eV(0) + 20k_B T$) are retained. In the following a bias $V(0) - V(L) = 0.25$ V and $T = 77$ K are used, so that about 6,700 eigenstates are considered. Scattering states are decomposed into right- and left-traveling states

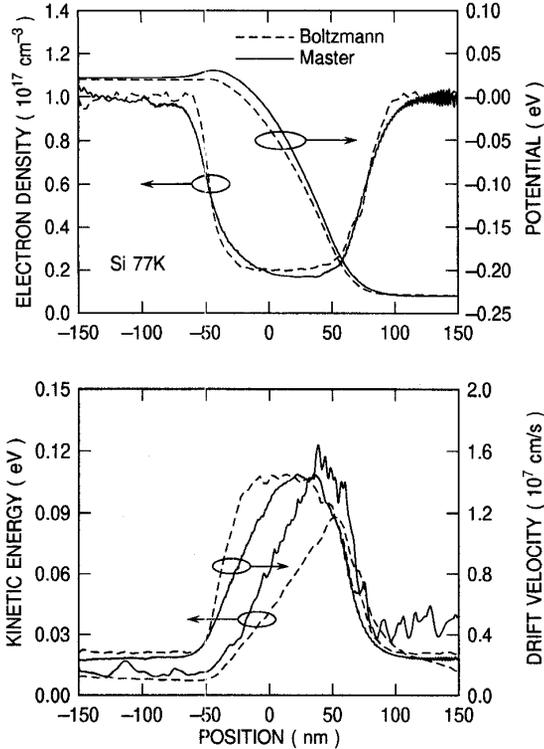


Figure 1: Calculated potential energy, electron charge density (top frame), average drift velocity and average kinetic energy (bottom frame) for the *nin* Si diode at 77 K described in the text, biased at 0.25 V. The solid lines refer to results calculated using the master equation, the dashed lines to results obtained a semiclassical full-band Monte Carlo simulation employing identical parameters.

($s = \mp$) by solving Eq. (11) with a fourth-order Runge-Kutta method. In the nondegenerate limit, for the open system considered here, and at steady state, Eq. (8) with the source term (9) takes the form of a linear problem:

$$\sum_{\lambda\kappa'r} \{W_{\mu\kappa s; \lambda\kappa'r} \rho_{\lambda\kappa'}^{(r)} - W_{\lambda\kappa'r; \mu\kappa s} \rho_{\mu\kappa}^{(s)}\} + |A_{\mu\kappa}^{(s)}|^2 v_z(\kappa, k_{\mu\kappa}^{(s)}) \rho_{\mu\kappa}^{(s)} = |A_{\mu\kappa}^{(s)}|^2 v_z(\kappa, k_{\mu\kappa}^{(s)}) f^{(s)}(k_{\mu\kappa}^{(s)} + k_{z,d}^{(s)}), \quad (12)$$

where the quantities $\rho_{\mu\kappa}^{(s)}$ stand for the diagonal elements of the reduced density matrix $\rho_{\mu\kappa s; \mu\kappa s}^{(el)}$, which are now assumed to be normalized so that $\sum_{\mu\kappa s} \rho_{\mu\kappa}^{(s)}$ is the electron density per unit area. The quasi-equilibrium distributions in the contacts, $f^{(s)}$, are obtained integrating the ‘drifted’ Fermi-Dirac distributions in each square in κ -space using the Gilat-Raubenheimer scheme presented above. The matrix on the left-hand-side of Eq. (12) can be inverted numerically. The linear problem is then solved while varying the source terms $f^{(s)}$ in order to satisfy the current continuity condition at the boundaries, using a Newton method to determine the required drift vector $k_{z,d}^{(s)}$. The result of the linear problem is then employed to solve the

Poisson equation. Finally, the new potential $V(z)$ is used to solve Eqns. (10) by Fourier transforms and (11) again, using under-relaxation schemes. The iteration is continued until a preset error condition on the L^2 -norm of the potential update is met (typically, 10^{-5} V).

The scattering processes considered are nonpolar interactions with transverse and longitudinal acoustic and optical phonons with the parameters described in Ref. [16]. The results of the simulation are shown in Fig. 1. On the top frame the self-consistent potential and electron density are shown and compared with the results obtained using a semiclassical Monte Carlo solution of the Boltzmann transport equation[14]. The differences are surprisingly small and can be attributed mostly to a different electrostatics. This is particularly evident in the increased height of the built-in potential barrier at the $n-i$ junction on the emitter side of the device. The bottom frame of Fig. 1 shows a comparison between the calculated electron average energy and drift velocity obtained using the Boltzmann and the master transport equations. These average quantities, somewhat ill-defined as they are functions of the position inside the structure, have been assigned a meaning by the procedure described in Ref. [2], with the obvious modifications dictated by the nonparabolic dispersion.

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