

Scattering in NEGF: Made simple

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Important definitions in the NEGF method

We start with a short re-statement of the main formulas for the Keldysh non-equilibrium Green's function method (NEGF). It is presumed that the reader is already familiar with it, see e.g. [1].

The device is described by, H , the device Hamiltonian and the self-energy functions Σ_c represent the semi-infinite ideal source/drain contacts. Σ_s is the self-energy for all mechanisms of scattering (e.g. spin relaxation, electron-phonon scattering)

$$\Sigma(E) = \Sigma_c(E) + \Sigma_s(E) \quad (1)$$

For a general classical description of scattering see [2]. The contact self energy is the sum of that for the source and the drain:

$$\Sigma_c(E) = \Sigma_s(E) + \Sigma_D(E) \quad (2)$$

The retarded Green's function for the device in the matrix form

$$G(E) = \left[(E + i\eta^+)I - H - \Sigma(E) \right]^{-1}$$

$$(3)$$

where η^+ is an infinitesimal positive value, and I the identity matrix.

The spectral function which is proportional to the density of states is defined as

$$A(E) = i(G(E) - G^\dagger(E)) = -2\text{Im}(G(E)) \quad (4)$$

where G^\dagger represents the Hermitian conjugate of G matrix. The spectral function is connected to the electron and hole correlation functions (see [1] Appendix) as follows

$$A(E) = G^n(E) + G^p(E) \quad (5)$$

The same set of relations exists between the sets of functions related to the Green's function G, G^n, G^p, A and related to the self energy $\Sigma, \Sigma^{in}, \Sigma^{out}, \Gamma$, as follows. Here, $\Sigma^{in/out}$ are the in/out-scattering functions. Level broadening is

$$\Gamma(E) = i[\Sigma(E) - \Sigma^\dagger(E)] = -2\text{Im}(\Sigma(E)), \quad (6)$$

$$\Gamma(E) = \Sigma^{in}(E) + \Sigma^{out}(E), \quad (7)$$

The retarded Green's function and the self energy are causal functions when transformed to time domain, i.e. they affect only the events in the future and thus are non-zero only for positive time. For such functions, the real and imaginary parts G^r, G^i are related by the Hilbert transform (these are also called Kramers-Kronig relations)

$$G^r(E) = -P \int \frac{dE'}{\pi} \frac{G^i(E')}{E - E'}, \quad (8)$$

$$G^i(E) = P \int \frac{dE'}{\pi} \frac{G^r(E')}{E - E'}. \quad (9)$$

And the same set of relations for Σ^r, Σ^i enables us to calculate the imaginary part from level broadening (P stands for the principal value of a singular integral)

$$\Sigma^r = P \int \frac{dE'}{2\pi} \frac{\Gamma(E')}{E - E'}. \quad (10)$$

The real part of self-energy is manifested as a shift of energy levels, and the imaginary part as their broadening. It also means that the imaginary part of self-energy is,

$$\Sigma^i(E) = -\frac{i}{2} \Gamma(E) = -\frac{i}{2} [\Sigma^{in}(E) + \Sigma^{out}(E)]. \quad (11)$$

The electron and hole correlation functions according to the reservoir theory (see [1] Chapter 11) are then given by,

$$G^n(E) = G \Sigma^{in} G^\dagger \quad (12)$$

$$G^p(E) = G \Sigma^{out} G^\dagger \quad (13)$$

Since physically sensible scattering functions are Hermitian

$$\Sigma^{in}(E) = \Sigma^{in\dagger}(E), \quad (14)$$

$$\Sigma^{out}(E) = \Sigma^{out\dagger}(E), \quad (15)$$

then the correlation functions are Hermitian too

$$G^n(E) = G^{n\dagger}(E), \quad (16)$$

$$G^p(E) = G^{p\dagger}(E). \quad (17)$$

The electron and hole densities in three dimensions are

$$n(r) = g_s g_v \frac{1}{a_x a_y a_z} \int_{-\infty}^{+\infty} \frac{G^n(r, r, E)}{2\pi} dE \quad (18)$$

$$p(r) = g_s g_v \frac{1}{a_x a_y a_z} \int_{-\infty}^{+\infty} \frac{G^p(r, r, E)}{2\pi} dE \quad (19)$$

where summation over the spin and degenerate valleys in the bands results in the factors $g_s = 2$ and g_v , respectively, r is the vector of the coordinates, and a are the cell sizes along each dimension. It can be either the lattice constant of a crystal in the atomistic representation, or a grid size in the continuous representation. In case grid is not rectangular, $a_x a_y a_z$ needs to be replaced by the volume of the unit cell.

Traditionally, the particle density is expressed via the electron and hole occupation numbers, $\langle n \rangle$ and $\langle p \rangle$, and the density of states density of states $g_D(E)$ where the index D stands for the number of dimensions

$$n = \int_{-\infty}^{+\infty} \langle n \rangle g_D(E) dE \quad (20)$$

$$p = \int_{-\infty}^{+\infty} \langle p \rangle g_D(E) dE \quad (21)$$

Thus in consideration of (5), we find that the electron and hole correlation functions are related to the occupation numbers of electrons and holes

$$\langle n(E) \rangle = G^n(E) / A(E), \quad \langle p(E) \rangle = G^p(E) / A(E) \quad (22)$$

and the spectral function is related to the density of states

$$g_D(E) = g_s g_v \frac{A(E)}{2\pi a^3} \quad (23)$$

Finally, the current flow from slice x_j to x_{j+1} in the case of nearest-neighbor tight-binding [3]

$$I_{j \rightarrow j+1} = g_s g_v \frac{ie}{\hbar} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \left[H_{j,j+1} G_{j+1,j}^n(E) - H_{j+1,j} G_{j,j+1}^n(E) \right]. \quad (24)$$

Note about units

It is of advantage to keep consistent units of main NEGF values even if the geometrical dimensions of the device change. The Hamiltonian, self-energies, and in- and out-scattering functions have the units of [energy]

$$[H] = [E] = [\Sigma] = [\Gamma] = J \quad (25)$$

The Green's functions and the correlation functions have the units of inverse energy, i.e., [1/energy]:

$$[G] = [A] = J^{-1} \quad (26)$$

Unlike these, the traditional physical quantities, like density or density of states, change their units depending on the geometrical dimension D of the device.

$$[n] = [p] = m^{-D}, \quad [g_D] = J^{-1} \cdot m^{-D} \quad (27)$$

We will specifically note if exceptions to these rules exist.

Transformation to another basis of functions

Here we derive general expressions for the transform of coordinates from all spatial dimensions to the basis of eigenfunctions along some dimensions. It is applicable to momentum states along the unconfined transverse dimensions. Moreover, we will apply it later to momentum state representation along confined transverse dimensions. We transform from the coordinate

representation to another basis of functions in the Hilbert space $\psi_n(r)$ enumerated by the index n . We ensure that these functions are orthogonal and normalized

$$\sum_r \psi_m^*(r) \psi_n(r) = \delta(m, n).$$

(28)

Then, by usual rules of linear algebra, a matrix of two spatial variables transforms as

$$\Sigma_{mn} = \sum_{r,r'} \psi_m^*(r) \Sigma(r, r') \psi_n(r').$$

(29)

And the inverse transformation for any matrix is

$$G(r, r') = \sum_{m,n} \psi_m(r) G_{mn} \psi_n^*(r'). \quad (30)$$

These rules will enable us to write the scattering function in any basis set of functions. Note that these sums do not contain the dimensional factors and thus do not change the units of the summed physical quantities.

Elastic scattering

In any case (like spin relaxation or elastic phonon scattering) when the in- and out-scattering energies being proportional to Green's functions at the same energy, the expression of the self energy drastically simplifies. If we know that

$$\Sigma_s^{in}(E) = \mathbf{D}(E)G^n(E), \quad \Sigma_s^{out}(E) = \mathbf{D}(E)G^p(E). \quad (31)$$

Then we easily obtain that

$$\Gamma(E) = \mathbf{D}(E)A(E), \quad \Sigma^i(E) = \mathbf{D}(E)G^i(E) \quad (32)$$

In case of the pre-factor varying slowly with energy, one can expand it into the Taylor series

$$\mathbf{D}(E') = \mathbf{D}(E) - (E - E')\mathbf{D}'(E) + \dots \quad (33)$$

Then the Hilbert transform (retaining only two terms in the series) is

$$\Sigma^r = \mathcal{P} \int \frac{dE'}{2\pi} \frac{\mathbf{D}(E')A(E')}{E - E'} \approx \mathcal{P} \int \frac{dE'}{2\pi} \frac{\mathbf{D}(E)A(E')}{E - E'} - \int \frac{dE'}{2\pi} \mathbf{D}'(E)A(E') = \mathbf{D}(E)G^r(E) - \mathbf{D}'(E)N_{st}, \quad (34)$$

where N_{st} is the total number of states. Thus if the pre-factor is constant or at least changes with energy slowly enough over the range of energies of interest, such that we can neglect the second term in the above equation, then we find that the self energy is proportional to the Green's function. To summarize

$$\Sigma_s^{in}(E) = \mathbf{D}G^n(E), \quad \Sigma_s^{out}(E) = \mathbf{D}G^p(E), \quad \Sigma_s(E) = \mathbf{D}G(E), \quad \Gamma(E) = \mathbf{D}A(E) \quad (35)$$

Spin relaxation

The spin relaxation tensor \mathbf{D} is calculated according to [4]. It is taken here to have the same functional form for electrons and holes.

We can explicitly write the spin indices, such that e.g. the diagonal blocks become

$$G = \begin{pmatrix} G_{uu} & G_{ud} \\ G_{du} & G_{dd} \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_{uu} & \Sigma_{ud} \\ \Sigma_{du} & \Sigma_{dd} \end{pmatrix} \quad (36)$$

The relaxation tensor can be separated into the coupling factor and the dimensionless tensor

$$\mathbf{D}(E) = D(E)\Phi. \quad (37)$$

For the case of isotropic relaxation, the dimensionless tensor is (see [4])

$$4\Phi_{ij11} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad 4\Phi_{ij12} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, \quad 4\Phi_{ij21} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \quad 4\Phi_{ij22} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}. \quad (38)$$

And the equation for the self energy turns to,

$$\Sigma_s = \frac{D}{4} \begin{pmatrix} G_{uu} + 2G_{dd} & -G_{ud} \\ -G_{du} & 2G_{uu} + G_{dd} \end{pmatrix}. \quad (39)$$

The spin scattering rate $\gamma(E)$ is proportional to the coupling factor

$$\Gamma(E) = \hbar\gamma(E) = D(E)A(E). \quad (40)$$

The spin scattering rate can be related to the spin-flip rate T_1^{-1} , which is more familiar to experimentalists, see [5]. The latter one refers to the rate averaged over the energy. In the case of two dimensions, density of states is constant, and the spin scattering rate is constant too, and coincides with the averaged over energies.

$$T_1^{-1}(E) = 2\gamma(E). \quad (41)$$

Spin flip rate contains an extra factor of 2, since it refers to the spin polarization rather than populations in the spin-up and spin-down states separately. The density of states is related to the spectral function as follows

$$g_{2D}(E) \equiv \frac{m}{\pi\hbar^2} = \frac{2A(E)}{2\pi a_x a_y}. \quad (42)$$

Thus the coupling constant can be expressed via the spin-flip rate

$$D(E) = \frac{\hbar^3}{2T_1 m a_x a_y}. \quad (43)$$

Self-consistent loops

To calculate the Green's functions and charge and current densities coming out of them, we need to solve non-linear equations. We prefer to solve them in an iterative manner, solving linear equations at every step of the iteration. The symbols with a bar designate the quantities from the previous step of iteration

$$\Sigma_s(E) = \mathbf{D}\bar{G}(E), \quad \Sigma_s^{in}(E) = \mathbf{D}\bar{G}^n(E) \quad (44)$$

$$G(E) = \left[(E + i\eta^+)I - H - \Sigma_c(E) - \Sigma_s(E) \right]^{-1} \quad (45)$$

$$G^n(E) = G(E) \left(\Sigma_c^{in}(E) + \Sigma_s^{in}(E) \right) G^\dagger(E) \quad (46)$$

Note that practically for block 3-diagonal matrices, the above two equations are not implemented as direct matrix multiplication, but rather as a recursive Green's function algorithm. The iteration

loop ends, when \bar{G} and G are sufficiently close according to some metric. Such a loop is done for every value on the energy grid. Then the charge density is calculated via Eqs. (18) and (19). The charge density is used in the outer loop with Poisson's equation.

Surface scattering in a quantum well

Here we consider surface roughness scattering in the quantum well with confinement along the z axis, transport direction x and the unconfined transverse dimension y.

We start with the semi-classical expression for the rate of surface roughness scattering [6]. The square of the Hamiltonian for scattering normalized per area with sizes L_x and L_y is

$$|H_{k,k'}|^2 = M^2 Y(k'-k) / (L_x L_y) \quad (47)$$

is expressed via the square of the matrix element (with the units of $(J \cdot m)^2$), which is for small [7] and large [8] quantum well thickness L_w , respectively,

$$M^2 = \pi \Delta^2 \Lambda^2 \frac{\pi^4 \hbar^4}{m^{*2} L_w^6} \quad \text{and} \quad M^2 = \pi \Delta^2 \Lambda^2 e^2 F_s^2, \quad (48)$$

where the correlation length is Λ , the roughness r.m.s. is Δ , and the effective normal field at interface is F_s , and the carrier confinement mass is m^* . And the dimensionless factor in the Fourier transform of the roughness correlation function can have, for example, of Gaussian form

$$Y(q) = \exp\left(-\frac{\Lambda^2 q^2}{4}\right). \quad (49)$$

Then the total rate of scattering of the of electrons with in-plane momentum k to all possible final momenta k' is then given by the Fermi's golden rule

$$\frac{1}{\tau(k)} = \frac{2\pi}{\hbar} \sum_{k'} |H_{k,k'}|^2 \delta(E_{k'} - E_k). \quad (50)$$

Now we can substitute the Hamiltonian and use the representation of the sum over the momentum states as an integral

$$\sum_{k'} = \frac{L_x L_y}{(2\pi)^2} \int d^2 k'. \quad (51)$$

Then the scattering rate becomes

$$\frac{1}{\tau(k)} = \frac{M^2}{2\pi\hbar} \int Y(q) \delta(E_{k'} - E_k) d^2 k'. \quad (52)$$

This rate should be distinguished from the momentum relaxation rate.

$$\frac{1}{\tau_m(k)} = \frac{M^2}{2\pi\hbar} \int Y(q) \delta(E_{k'} - E_k) (1 - \cos\theta) d^2 k'. \quad (53)$$

Here the exchange of in-plane momentum is $q = k' - k$, and θ is the angle between the momenta k', k . By expressing the differential of energy via the momentum magnitude

$$dE = \frac{\hbar^2 k' dk'}{m_d}, \quad (54)$$

where m_d is the density-of-states mass. Performing the integral over energies which results in a unity factor

$$\frac{1}{\tau_m(k)} = \frac{m_d M^2}{\hbar^3} \cdot \frac{1}{2\pi} \int_0^{2\pi} d\theta (1 - \cos\theta) Y(q). \quad (55)$$

Note that for small correlation length $Y(q) = 1$ (isotropic scattering), the last factor in the above equation turns to unity, and the total scattering rate becomes equal to the momentum relaxation rate. This limit is valid when most of electrons have momentum such that $k\Lambda \ll 1$. For non-degenerate carriers, the characteristic momentum is given by the thermal velocity

$$v_t = \sqrt{\frac{2k_B T}{\pi m_c}} \approx 120 \text{ km/s}. \quad (56)$$

and thus this momentum is

$$k_t = \frac{m_d v_t}{\hbar} \approx 0.2 \text{ nm}^{-1}. \quad (57)$$

Therefore the approximation valid to a correlation length of a couple of nanometers.

The part of mobility limited by surface roughness scattering contains the averaged scattering time and the conduction mass m_c .

$$\mu_{srs} = \frac{e \langle \tau_m \rangle}{m_c} . \quad (58)$$

For sufficiently wide quantum wells, one retrieves the well-known ‘universal mobility’ dependence

$$\mu_{srs} \propto \frac{1}{F_s^2} . \quad (59)$$

In the isotropic limit the scattering rate is

$$\frac{1}{\tau} = \frac{m_d M^2}{\hbar^3} . \quad (60)$$

And the mobility becomes

$$\mu_{iso} = \frac{e \hbar^3}{m_c m_d M^2} . \quad (61)$$

We see that mobility decreases with correlation length in the isotropic limit

$$\mu_{iso} \propto \Lambda^{-2} . \quad (62)$$

The intuitive explanation for this is that electrons diffract around roughness which is smaller than their wavelength and do not get scattered by it.

In the opposite limit of long correlation length, the angle-dependent factor is

$$\int_0^{2\pi} d\theta (1 - \cos \theta) Y(q) \approx \frac{2\sqrt{\pi}}{(k\Lambda)^3}. \quad (63)$$

and therefore mobility increases with correlation length:

$$\mu \propto \Lambda. \quad (64)$$

The intuitive explanation for this is that when the correlation length is longer than the wavelength of electrons, they are able to adiabatically adjust to the changes in the waveguide width and not to experience scattering.

When fitting the experimental data, the r.m.s. roughness and the correlation length are not well know. Therefore it is necessary to fit the value of mobility, which is easier to obtain. For example, for electrons in silicon, $\Delta = 0.5nm$, $\Lambda = 2nm$, and $F_s = 1MV/cm$ would produce the matrix element of $M = 0.177eV \cdot nm$, scattering rate of $\tau^{-1} = 2.0 \cdot 10^{14}/s$ and mobility

$$\mu_{iso} = 44 \frac{cm^2}{V \cdot s}.$$

Now we draw the connection between the semi-classical scattering rate and the full quantum description via NEGF. In the NEGF formalism, the surface scattering has the form of the broadening function for elastic process with transfer of momentum expressed via the spectral function, that is

$$\Gamma(k_x, k_x', k_y, k_y', E) = \frac{1}{N_x N_y} \sum_q K_s Y(q) A(k_x + q_x, k_x' + q_x, k_y + q_y, k_y' + q_y, E)$$

(65)

Here we separated the scattering prefactor into a constant K_s (with units of J^2) and the dimensionless factor of the correlation function $Y(q)$.

For 2-dimensional systems, the spectral function A

$$A(E_{k'}) = g_{2D}(E_{k'}) \pi a_x a_y. \quad (66)$$

Is related to the local density of states (LDOS)

$$g_{2D} = \frac{m_d}{\pi \hbar^2}. \quad (67)$$

Taking the special case of isotropic scattering, we can obtain the relation between the constants which is valid for the general case. In this case the scattering broadening

$$\Gamma = \frac{1}{N_x N_y} \sum_q K_s A = K_s A = \frac{K_s m_d a_x a_y}{\hbar^2}. \quad (68)$$

On the other hand the broadening is related to the scattering rate

$$\Gamma = \frac{\hbar}{\tau} = \frac{m_d M^2}{\hbar^2}. \quad (69)$$

A comparison of these expressions demands that

$$K_s = \frac{M^2}{a_x a_y}. \quad (70)$$

Now we need to transform the broadening function and the spectral function to real coordinates along the transport direction x according to Eqs. (28) and (29).

$$\Gamma(x_1, x_2) = \frac{1}{N_x} \sum_{k_x, k_x'} \Gamma(k_x, k_x') \exp(ik_x x_1 - ik_x' x_2) \quad (71)$$

$$A(k_x, k_x') = \frac{1}{N_x} \sum_{x_3, x_4} A(x_3, x_4) \exp(ik_x' x_4 - ik_x x_3) \quad (72)$$

Upon substitution of these equations to (65), performing summation over momenta according to the identity

$$N_x \delta(x_1, x_3) = \sum_{k_x} \exp(ik_x x_1 - ik_x x_3), \quad (73)$$

and performing summation with Kronecker delta symbols under the sums, we obtain

$$\Gamma(x_1, x_2, k_y, k_y', E) = \frac{K_s}{N_x N_y} \sum_q Y(q) A(x_1, x_2, k_y + q_y, k_y' + q_y, E) \exp(iq_x x_2 - iq_x x_1), \quad (74)$$

At this point we neglect correlations between the transverse momenta, and treat them as a set of independent modes by dropping the second momentum variable in all functions as follows $\Gamma(x_1, x_2, k_y, E)$. Taking advantage of the fact that this particular form of the roughness correlation admits splitting into a product $Y(q) = Y(q_x)Y(q_y)$, we can perform summation over the transferred x -momentum

$$I_{trx} = \sum_{q_x} \exp\left(-\frac{\Lambda^2 q_x^2}{4}\right) \exp(iq_x \Delta x) = \frac{L_x}{\Lambda \sqrt{\pi}} \exp\left(-\frac{\Delta x^2}{\Lambda^2}\right). \quad (75)$$

Now we would like to perform summation over the transverse momenta and will limit ourselves to cases where the Green's function is approximately independent of the transverse momentum (and thus can be taken out of the summation). Then the summation over transferred y-momentum is performed similarly, to yield

$$\Gamma(x_1, x_2, E) = C_s \exp\left(-\frac{(x_2 - x_1)^2}{\Lambda^2}\right) A(x_1, x_2, E). \quad (76)$$

$$C_s = \frac{M^2}{\pi \Lambda^2} = 2.5 \cdot 10^{-3} eV^2. \quad (77)$$

Other scattering related functions, $\Sigma, \Sigma^{in}, \Sigma^{out}$, have the same dependence on the coordinates and the functional form the Green's functions enter the equations, e.g.

$$\Sigma(x_1, x_2, E) = C_s \exp\left(-\frac{(x_2 - x_1)^2}{\Lambda^2}\right) G(x_1, x_2, E). \quad (78)$$

Not surprisingly, the broadening function contains the spatial correlation function of roughness. However with this dependence, the broadening, self-energy matrices, as well as the whole NEGF equations become strongly non-diagonal. Instead of the desired one sub-diagonal and one super-diagonal, their number is equal to the ratio of the correlation length and the spatial grid size Λ/a_x , which can be >30 . That would drastically increase the computational burden of solving these equations. Therefore we will be looking for an approximation that would permit us to express off-diagonal elements of the Green's function via the 3-diagonal ones. The scattering

terms in the equation (3) for the Green's function, originating from the matrix multiplication ΣG , have the form

$$ST(x_1, x_3, E) = \sum_{x_2} \Sigma(x_1, x_2, E) G(x_2, x_3, E). \quad (79)$$

From the direct solution of the full-matrix equations of the Green's function one can see that it typically has the damped oscillatory dependence on the coordinates, which can be approximated by an exponential dependence with a complex κ

$$G(x_1, x_2, E) = G(x_2, x_1, E) = G(x_1, x_1, E) \exp(\kappa |x_2 - x_1|). \quad (80)$$

Substituting an expression for the self-energy with an arbitrary prefactor C_s

$$ST(x_1, x_3, E) = C_s \sum_{x_2} \exp\left(-\frac{(x_2 - x_1)^2}{\Lambda^2}\right) G(x_1, x_2, E) G(x_2, x_3, E), \quad (81)$$

using the approximation for the Green's function

$$\begin{aligned} ST(x_1, x_3, E) &= C_s G(x_1, x_1, E) G(x_3, x_3, E) \\ &\times \sum_{x_2} \exp\left(-\frac{(x_2 - x_1)^2}{\Lambda^2}\right) \exp(\kappa |x_1 - x_2|) \exp(\kappa |x_2 - x_3|). \end{aligned} \quad (82)$$

In the following, only consider a uniform grid $x_i = a_x n_i$. In this case the exponent of the Green's function is easily calculated from just the diagonal and the first super-diagonal terms

$$G(n_1, n_1 + 1, E) / G(n_1, n_1, E) = \exp(\kappa a_x) \quad (83)$$

The scattering terms become

$$ST(x_1, x_3, E) = C_s G(x_1, x_1, E) G(x_3, x_3, E) \times \left[\begin{aligned} & \sum_{n_2 \geq n_3} \exp\left(-\frac{a_x^2 (n_2 - n_1)^2}{\Lambda^2}\right) \exp(2\kappa a_x n_2 - \kappa a_x n_1 - \kappa a_x n_3) \\ & + \sum_{n_2 < n_3} \exp\left(-\frac{a_x^2 (n_2 - n_1)^2}{\Lambda^2}\right) \exp(\kappa a_x n_1 + \kappa a_x n_3 - 2\kappa a_x n_2) \end{aligned} \right] \quad (84)$$

Focusing for simplicity on diagonal scattering terms only:

$$ST(x_1, x_1, E) = C_s G^2(x_1, x_1, E) \left[1 + 2 \sum_{n_2 > n_1} \exp\left(-\frac{a_x^2 (n_2 - n_1)^2}{\Lambda^2}\right) \exp(2\kappa a_x (n_2 - n_1)) \right] \quad (85)$$

In other words, the scattering terms are approximated by an expression containing 3-diagonal terms of the Green's function only (rather than more distant diagonals of it)

$$\Sigma(x_1, x_1, E) = C_s F_{cor} G(x_1, x_1, E) \quad (86)$$

where the correlation factor

$$F_{cor}(\Lambda, G(n_1, n_1 + 1, E) / G(n_1, n_1, E)) = 1 + 2 \sum_{n_2 > n_1} \exp\left(-\frac{a_x^2 (n_2 - n_1)^2}{\Lambda^2}\right) \exp(2\kappa a_x (n_2 - n_1)) \quad (87)$$

This is not a material constant, it varies with energy and coordinates! Further approximations depend on the correlation length. If it is comparable with the device size $\Lambda \sim L_x$, no diagonal approximation makes sense. If the correlation length is smaller than the device size, but larger

than the grid size $a_x \ll \Lambda \ll L_x$, the sum can be well approximated by an integral with limits extended to infinity. If the correlation length is comparable to the grid size $\Lambda \sim a_x$, the integral approximation is not valid and it is necessary to evaluate the sum above directly, which is a more general and preferred way.

$$F_{cor} = 1 + 2 \int_0^\infty \exp\left(-\frac{a_x^2 n^2}{\Lambda^2}\right) \exp(2\kappa a_x n) dn. \quad (88)$$

The integral can be explicitly obtained using a general derivation

$$\begin{aligned} \int_0^\infty \exp(-a^2 n^2 + 2bn) dn &= \int_0^\infty \exp(-a^2 n^2 + 2anb/a - b^2/a^2 + b^2/a^2) dn \\ &= \exp(b^2/a^2) \int_0^\infty \exp(-(an - b/a)^2) dn = \frac{1}{a} \exp(b^2/a^2) \int_{-b/a}^\infty \exp(-m^2) dm. \quad (89) \\ &= \frac{\sqrt{\pi}}{2a} \exp(b^2/a^2) \operatorname{erfc}(-b/a) \end{aligned}$$

which results in

$$F_{cor} = 1 + \frac{\Lambda \sqrt{\pi}}{a_x} \exp(\kappa^2 \Lambda^2) \operatorname{erfc}(-\kappa \Lambda). \quad (90)$$

This results in a convenient expression for surface scattering which can be tested against other simulation methods. For the above roughness parameters, $a_x = 0.4nm$, and $\kappa = -1/5nm$ one obtains the constant $F_{cor} = 6.9$. Note that in the case when one of the transverse dimensions is confined, the rates of scattering between various subbands must contain the formfactors, as described below.

General expression for electron-phonon self-energy

Electron-phonons scattering included as in- and out-scattering functions. In the self consistent first Born approximation they are

$$\Sigma^{in,out}(X_1, X_2) = D^{n,p}(X_1, X_2)G^{n,p}(X_1, X_2). \quad (91)$$

where the argument $X = \{r, t\}$ incorporates the spatial coordinates (both confined and unconfined), and time, respectively. This is graphically expressed as the “sunrise” Feynman diagram (Figure 1).

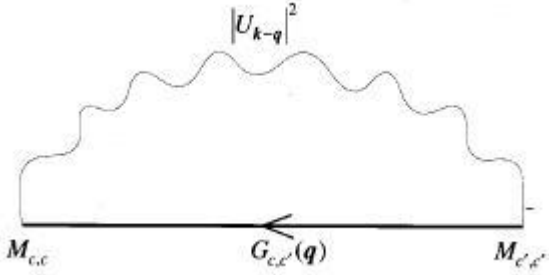


FIG. 1. Feynman diagram for the first self-consistent Born approximation of phonon scattering.

The phonon propagator contains the average over the random variables of the phonon reservoir designated by angle brackets,

$$D^n(X_1, X_2) = \langle H_{ep}(X_1)H_{ep}(X_2) \rangle, \quad D^p(X_1, X_2) = \langle H_{ep}(X_2)H_{ep}(X_1) \rangle \quad (92)$$

Here the electron-phonon interaction Hamiltonian is

$$H_{ep} = \sum_q M_q a_q \left(b_q e^{-i\omega_q t + iqr} + b_q^\dagger e^{i\omega_q t - iqr} \right) \quad (93)$$

where b_q^\dagger, b_q are the creation and annihilation operators for phonons in the mode q , and the half-amplitude for one phonon in the total device volume V with density ρ is

$$a_q = \sqrt{\frac{\hbar}{2\rho V \omega_q}} \quad (94)$$

The units of the matrix element M_q is [energy/length] and of the units of the half-amplitude a_q is [length]. The summation over momentum states will be performed over functions which are periodic in the reciprocal lattice and is generally defined via a dimensionless integral over the first Brillouin zone,

$$\sum_q = \left(\frac{L}{2\pi}\right)^D \int d^D q. \quad (95)$$

where D is the number of dimensions over which the momentum is summed, L are sizes along these dimensions, so that the volume in these dimensions is $V = L^D$. The sum is normalized to $(L/a)^D = N$, number of lattice unit cells, where a is the cell size. The summation of the exponent over the first Brillouin zone, where the coordinates belong to the Bravais lattice (note that spatial coordinates are discretized) gives the delta function (see e.g. Appendix D in [9]). It can be easily verified directly in the case of a uniform 1D lattice. Similarly the summation over the coordinate is performed over all lattice cells and contains the normalization factor N . Thus

$$\sum_q \exp(iqr) = N\delta(r). \quad (96)$$

$$\sum_r \exp(iqr) = N\delta(q). \quad (97)$$

Note that these sums do not contain the dimensional factors and thus do not change the units of the summed physical quantities. The averages of the operator products in a reservoir at thermal equilibrium with temperature T depend on the phonon occupation numbers for each mode with momentum q , and energy ω_q

$$n_q = \left(\exp\left(\frac{\hbar\omega_q}{k_B T}\right) - 1 \right)^{-1}. \quad (98)$$

such that

$$\langle b_q^\dagger b_{q'} \rangle = \delta_{qq'} n_q, \quad \langle b_q b_q^\dagger \rangle = \delta_{qq'} (n_q + 1), \quad (99)$$

and all other averages of pair products are zero.

On substitution of the electron-phonon Hamiltonian (93) it results in,

$$D^n(r_1, t_1, r_2, t_2) = \sum_q |M_q|^2 a_q^2 \left[(n_q + 1) \exp(i\omega_q(t_2 - t_1) + iq(r_1 - r_2)) + n_q \exp(i\omega_q(t_1 - t_2) + iq(r_2 - r_1)) \right] \quad (100)$$

and a similar expression for $D^p(r_1, t_1, r_2, t_2)$.

Then we limit the consideration to stationary situation, i.e. where the functions depend only on the difference of times $t = t_2 - t_1$. The Fourier transform relative to this time interval

$$\Sigma^{in}(E) = \frac{1}{2\pi} \int dt e^{iEt} \Sigma^{in}(t_1, t_2), \quad (101)$$

which produces energy-dependent in/out-scattering functions,

$$\boxed{\Sigma^{in}(r_1, r_2, E) = D(r_1, r_2, E) (n_q + 1) G^n(r_1, r_2, E + \hbar\omega_q) + D^*(r_1, r_2, E) n_q G^n(r_1, r_2, E - \hbar\omega_q)} \quad (102)$$

$$\boxed{\Sigma^{out}(r_1, r_2, E) = D^*(r_1, r_2, E) (n_q + 1) G^p(r_1, r_2, E - \hbar\omega_q) + D(r_1, r_2, E) n_q G^p(r_1, r_2, E + \hbar\omega_q)} \quad (103)$$

where the first term in the expressions corresponds to emission of a phonon, and the second one – to absorption of a phonon. The electron-phonon coupling operator contains the sum over the phonon momentum that operates on the factors to the right of it,

$$D(r_1, r_2, E) = \sum_q |M_q|^2 a_q^2 \exp(iq(r_1 - r_2)) \quad (104)$$

It depends on the difference of the spatial coordinates $r = r_2 - r_1$.

Unconfined dimensions

From this point on, we would like to treat the unconfined spatial dimensions differently. We split the coordinates into the unconfined transverse and all other projections $r = \{r_i, r_l\}$. Similarly we split the momentum into the projections along the unconfined transverse dimensions and all other projections $q = \{q_i, q_l\}$. We will designate the number of confined and transport

dimensions as C , and the number of unconfined transverse dimensions as U . We clarify it for specific cases in Table 1.

Structure	No. confined dimensions, C $= 3-U$	Unconfined transverse dimensions	Transport and confined dimensions
Nanowire, quantum dot, molecule, tri-gate transistor	3		x, y, z
Ultra-thin body, planar transistor	2	z	x, y
Transport perpendicular to heterostructures (e.g. resonant tunneling diode)	1	y, z	x
Bulk solid state	0	x, y, z	

TABLE 1. Specification of dimensions for various transport structures.

We will be using the following relations pertaining to the split into the confined and unconfined dimensions. The total volume of the device is represented as the product of the confined and unconfined volumes, and similarly, the product of the grid sizes and the number of cells

$$V = V_{con} V_{unc} \quad (105)$$

$$a^3 = a_x a_y a_z = a^U a^C \quad (106)$$

$$N = N_{con} N_{unc} \quad (107)$$

The number of cells is related to the volume and the grid size.

$$V = N a^3, \quad V_{con} = N_{con} a^C, \quad V_{unc} = N_{unc} a^U \quad (108)$$

The expressions for the density relative to confined dimensions are also modified

$$n = g_s g_v \frac{1}{a^{3-U} V_{unc}} \sum_{kt} \int_{-\infty}^{+\infty} \frac{G^n(E)}{2\pi} dE \quad (109)$$

$$p = g_s g_v \frac{1}{a^{3-U} V_{unc}} \sum_{kt} \int_{-\infty}^{+\infty} \frac{G^p(E)}{2\pi} dE \quad (110)$$

With the transverse and longitudinal dimensions explicitly written

$$\begin{aligned} \Sigma^{in}(r_{1l}, r_{2l}, r_{1t}, r_{2t}, E) &= \sum_{ql, qt} |M_q|^2 a_q^2 \exp(iq_l(r_{1l} - r_{2l}) + iq_t(r_{1t} - r_{2t})) \\ &\times (n_q + 1) G^n(r_{1l}, r_{2l}, r_{1t}, r_{2t}, E + \hbar\omega_q) \\ &+ \sum_{ql, qt} |M_q|^2 a_q^2 \exp(-iq_l(r_{1l} - r_{2l}) - iq_t(r_{1t} - r_{2t})) \\ &\times n_q G^n(r_{1l}, r_{2l}, r_{1t}, r_{2t}, E - \hbar\omega_q) \end{aligned} \quad (111)$$

And similarly for the out-scattering function.

Scattering in momentum states representation

We switch to the momentum representation for the unconfined transverse dimensions by projecting to the momentum states (in this case, plane waves) which are normalized

$$\psi_k(r) = N^{-1/2} \exp(ikr), \quad (112)$$

where N is the number of grid cells, as follows

$$G^n(r_{1l}, r_{2l}, r_{1t}, r_{2t}, E) = N^{-1} \sum_{k'_{1t}, k'_{2t}} \exp(ik'_{1t} r_{1t} - ik'_{2t} r_{2t}) G^n(r_{1l}, r_{2l}, k'_{1t}, k'_{2t}, E) \quad (113)$$

$$\Sigma^{in}(r_{1l}, r_{2l}, k_{1t}, k_{2t}, E) = N^{-1} \sum_{r_{1t}, r_{2t}} \exp(-ik_{1t} r_{1t} + ik_{2t} r_{2t}) \Sigma^{in}(r_{1l}, r_{2l}, r_{1t}, r_{2t}, E) \quad (114)$$

Therefore the transformed in-scattering function is

$$\begin{aligned}
\Sigma^{in}(r_{1l}, r_{2l}, k_{1t}, k_{2t}, E) &= N^{-2} \sum_{r_{1t}, r_{2t}} \exp(-ik_{1t}r_{1t} + ik_{2t}r_{2t}) \\
&\sum_{q_l, q_t} |M_q|^2 a_q^2 \exp(iq_l(r_{1l} - r_{2l}) + iq_t(r_{1t} - r_{2t})) \\
&\times (n_q + 1) \sum_{k'_{1t}, k'_{2t}} \exp(+ik'_{1t}r_{1t} - ik'_{2t}r_{2t}) G^n(r_{1l}, r_{2l}, k'_{1t}, k'_{2t}, E + \hbar\omega_q) \\
&+ \text{absorption}
\end{aligned} \tag{115}$$

Performing summation over transverse coordinates and momenta,

$$\begin{aligned}
\Sigma^{in}(r_{1l}, r_{2l}, k_{1t}, k_{2t}, E) &= \sum_{q_l, q_t} |M_q|^2 a_q^2 (n_q + 1) \exp(iq_l(r_{1l} - r_{2l})) \\
&\times \sum_{k'_{1t}, k'_{2t}} \delta(-k_{1t} + q_t + k'_{1t}) \delta(k_{2t} - q_t - k'_{2t}) G^n(r_{1l}, r_{2l}, k'_{1t}, k'_{2t}, E + \hbar\omega_q). \\
&+ \text{absorption}
\end{aligned} \tag{116}$$

Here the delta functions express the momentum conservation for transverse momenta, $k = q_t + k'$, where k' is the transverse projection of momentum before scattering and k is the projection of momentum after scattering. Now we neglect the correlations between different states of transverse momentum, i.e. only retaining terms with $k'_1 = k'_2$ in the electron correlation function G^n . That results in the in-scattering function diagonal in transverse momentum states:

$$\boxed{
\begin{aligned}
\Sigma^{in}(r_1, r_2, k_t, E) &= \sum_{q_l, q_t} |M_q|^2 a_q^2 (n_q + 1) \exp(iq_l(r_1 - r_2)) G^n(r_1, r_2, k_t + q_t, E + \hbar\omega_q) \\
&+ \sum_{q_l, q_t} |M_q|^2 a_q^2 n_q \exp(-iq_l(r_1 - r_2)) G^n(r_1, r_2, k_t - q_t, E - \hbar\omega_q)
\end{aligned}
} \tag{117}$$

$$\Sigma^{out}(r_1, r_2, k_t, E) = \sum_{ql, qt} |K_q|^2 a_q^2 (n_q + 1) \exp(iq_l(r_1 - r_2)) G^p(r_1, r_2, k_t - q_t, E - \hbar\omega_q) + \sum_{ql, qt} |K_q|^2 a_q^2 n_q \exp(-iq_l(r_1 - r_2)) G^p(r_1, r_2, k_t + q_t, E + \hbar\omega_q) \quad (118)$$

And from here on we drop subscripts l of the coordinates. Note that the explicit coordinate dependence is only in the exponent containing longitudinal coordinates. As a sanity check, for zero unconfined dimensions these expressions reduce to (102) and (103). In the case of bulk (all dimensions unconfined) these expressions reduce to

$$\Sigma^{in}(k, E) = \sum_q |M_q|^2 a_q^2 (n_q + 1) G^n(k + q, E + \hbar\omega_q) + \sum_q |M_q|^2 a_q^2 n_q G^n(k - q, E - \hbar\omega_q), \quad (119)$$

$$\Sigma^{out}(k, E) = \sum_q |M_q|^2 a_q^2 (n_q + 1) G^p(k - q, E - \hbar\omega_q) + \sum_q |M_q|^2 a_q^2 n_q G^p(k + q, E + \hbar\omega_q). \quad (120)$$

The terms within the summation signs are equivalent to the scattering rates from (2.61) of [2]. The four cases of phonon scattering are considered below and corresponding matrix elements are taken from (2.59) of [2].

Four specific cases of phonon scattering

The expressions for the in/out-scattering functions drastically simplify in the two following cases. First, for isotropic scattering with phonons of constant energy ($|M_q| \approx D_o$ and $\omega_q \approx \omega_0$, and they are independent of q). This is approximately fulfilled for optical phonons and deformation potential interaction in non-polar crystals. In this case, the electron-phonon scattering operator reduces to calculation of a sum,

$$D(r_1, r_2, E) = \frac{\hbar D_o^2}{2\rho\omega_0} \frac{1}{V} \sum_{ql} \exp(iq_l(r_1 - r_2)), \quad (121)$$

According to (96), the sum in the above equation gives a Kronecker delta of the grid coordinates. This leads to a profound conclusion of the scattering operator being approximately local in the coordinate space:

$$D(r_1, r_2, E) = \frac{\hbar D_o^2 N_{con}}{2\rho\omega_0 V} \delta(r_1, r_2), \quad (122)$$

We will define the coupling constant of phonon scattering in a general manner involving the grid sizes of all three dimensions

$$K_o = \frac{\hbar D_o^2}{2\rho\omega_0 a^3}. \quad (123)$$

A general relation that we will encounter in all phonon self-energy calculations is

$$\frac{N_{con} a^3}{V} = \frac{V_{con} a^3}{V a^C} = \frac{a^U}{V_{unc}}. \quad (124)$$

Here a is the cell size, C is the number of confined dimensions, $U=3-C$ is the number of unconfined dimensions. Thus the phonon scattering operator is

$$D(r_1, r_2, E) = K_o \frac{a^U}{V_{unc}} \delta(r_1, r_2) \quad (125)$$

In other words, the in-scattering function is

$$\begin{aligned} \Sigma^{in}(r_1, r_1, k, E) &= K_o (n_0 + 1) \frac{a^U}{V_{unc}} \sum_{qt} G^n(r_1, r_1, k + q_t, E + \hbar\omega_0) \\ &+ K_o n_0 \frac{a^U}{V_{unc}} \sum_{qt} G^n(r_1, r_1, k - q_t, E - \hbar\omega_0) \end{aligned} \quad (126)$$

A very important conclusion is that the self-energy and the in/out-scattering functions can be treated as diagonal in this case. This significantly simplifies the problem and permits the use of various algorithms of solution of the matrix equations only applicable to 3-diagonal matrices, such as the recursive inversion method.

A connection can be made between the above in/out-scattering functions and the scattering rates traditionally used in classical scattering theories (like the Boltzmann equation and Monte Carlo methods of solution). For this the terms corresponding to emission and absorption of phonons need to be treated separately. We will limit the consideration here to the case of three unconfined dimensions, i.e. a bulk solid. Using the general rule that the broadening

$$\Gamma = \frac{\hbar}{\tau} \quad (127)$$

is related to the scattering time τ , the connection we must draw is

$$\Sigma_{em}^{in}(k, E) = \frac{\hbar}{\tau_{em}} \frac{a^U}{V_{unc}} \sum_{qt} \langle n \rangle (k + q_t, E + \hbar\omega_0). \quad (128)$$

Then (using (22) and the fact that the spectral function is independent of the transverse momentum) the scattering rate with emission is

$$\frac{1}{\tau_{em}}(E) = \frac{1}{\hbar} K_o (n_0 + 1) A(E + \hbar\omega_0). \quad (129)$$

upon substituting Eq. (23), which contains the factor of 2 for spin degeneracy, the rate becomes

$$\frac{1}{\tau_{em}}(E) = \frac{\pi D_o^2}{2\rho\omega_0}(n_0 + 1)g_{3D}(E + \hbar\omega_0), \quad (130)$$

which coincides with Eq. (2.98) of the book [2].

The second case is scattering by deformation potential, for example, acoustic phonons in non-polar crystals. We will argue that this scattering can be approximated as elastic, i.e., one can neglect the energy of a phonon compared to characteristic energy differences in the problem. For a small energy of a phonon, $\hbar\omega_q \ll k_B T$, the occupation number (98) can be approximated by a linear term and proves to be much larger than unity

$$n_q \approx \frac{k_B T}{\hbar\omega_q} \gg 1. \quad (131)$$

Then the expression for absorption processes becomes a complex conjugate to that for emission processes.

$$\Sigma^{in}(r_1, r_2, k, E) = \sum_{q^l, q^l} |M_q|^2 a_q^2 \exp(iq_l(r_1 - r_2)) n_q G^n(r_1, r_2, k, E) + c.c. \quad (132)$$

It is easy to see that only states with such high occupation number contribute significantly to the scattering self energy, and we can neglect scattering by more energetic phonons. The condition of small energy translates into small momentum of a phonon compared to the maximum phonon energy. For acoustic phonons with momentum of only a fraction of the edge of the Brillouin zone, we can take the dominant, linear terms in the dependence of energy and the coupling

matrix element on momentum: $\omega_q \approx v_a q$ and $|M_q| \approx D_a q$. The units of these new constants D_a is [energy].

$$\Sigma^{in}(r_1, r_2, k, E) = \sum_{ql, qt} D_a^2 q^2 \frac{k_B T}{\hbar \omega_q} \frac{\hbar}{2\rho V \omega_q} \exp(iq_l(r_1 - r_2)) G^n(r_1, r_2, k, E) + c.c.. \quad (133)$$

Then again as in (121), the product of the matrix element and the number of phonon proves to be independent of the phonon momentum and can be taken out of the summation. Since none of the terms under the sum depend on the transverse momentum, the summation over transverse momentum produces the factor N_{unc} .

$$\Sigma^{in}(r_1, r_2, k, E) = \frac{D_a^2 k_B T}{2\rho v_a^2} \frac{N_{unc}}{V} \sum_{ql} \exp(iq_l(r_1 - r_2)) G^n(r_1, r_2, k, E) + c.c.. \quad (134)$$

The summation over the longitudinal phonon momentum does not involve the electron momentum, and therefore, as before it produces a Kronecker delta factor

$$\Sigma^{in}(r_1, r_2, k, E) = \frac{D_a^2 k_B T}{2\rho v_a^2} \frac{N_{unc}}{V} N_{con} \delta(r_1, r_2) G^n(r_1, r_2, k, E) + c.c.. \quad (135)$$

The coupling constant for the acoustic phonons is

$$K_a = \frac{D_a^2 k_B T}{\rho v_a^2 a^3}. \quad (136)$$

And the resulting in-scattering function is

$$\Sigma^{in}(r_1, r_1, k, E) = K_a G^n(r_1, r_1, k, E). \quad (137)$$

Again this yields a diagonal in/out-scattering functions. Note an additional factor of 2 in these expressions because the processes with emission and absorption of a phonon are now lumped into one term. In any case (like above) of the in and out-scattering energies depending on the Green's functions at the same energy, the calculation of the self energy drastically simplifies (as we derived in Eq. (35)) and yields:

$$\Sigma^{in}(E) = K_a G^n(E), \quad \Sigma^{out}(E) = K_a G^p(E), \quad \Sigma(E) = K_a G(E). \quad (138)$$

Here we suppressed all coordinate and momentum variables to emphasize that the rule is general.

We can also draw the connection between these in/out-scattering functions and the classical scattering rates

$$\Sigma^{in}(k, E) = \frac{\hbar}{\tau} \langle n \rangle. \quad (139)$$

Repeating the same steps as for the optical phonon scattering, we identify the rate

$$\frac{1}{\tau}(E) = \frac{1}{\hbar} K_a A(E). \quad (140)$$

upon substituting (23), the rate becomes

$$\frac{1}{\tau}(E) = \frac{\pi D_a^2 k_B T}{\hbar \rho v_a^2} g_{3D}(E). \quad (141)$$

which coincides with Eq. (2.84) of the book [2].

Other cases are not as simple. For acoustic phonons in polar crystals, the piezo-electric coupling yields

$$M_{PZ} = \frac{e \cdot e_{PZ}}{\epsilon_s \epsilon_0}, \quad (142)$$

which is independent of the momentum. Then the in-scattering function is

$$\Sigma^{in}(r_1, r_2, k, E) = \frac{M_{PZ}^2 k_B T}{2\rho v_a^2 a} G^n(r_1, r_2, k, E) \frac{a}{V} \sum_{q_l, q_t} \exp(iq_l(r_1 - r_2)) q^{-2} + c.c. \quad (143)$$

We will consider only the case of no unconfined transverse dimensions and will leave other cases as homework for the reader ☺ ☺ ☺. The sum in this expression is proportional to the dimensionless integral over the first Brillouin zone.

$$I(r) = a \int_B \frac{\exp(iqr \cos \theta)}{q^2} d^3q. \quad (144)$$

where θ is the angle between the difference of coordinates and a variable momentum. We approximately calculate it over the spherically symmetric region with maximum momentum $q_m = 2\pi/a$.

$$I(r) \approx a \int_0^{q_m} dq 2\pi \int_{-1}^1 \exp(iqr \cos \theta) d \cos \theta = \int_0^{q_m} dq 4\pi \text{sinc}(qr). \quad (145)$$

This integral is approximately

$$I(r) \approx \begin{cases} 8\pi^2, & \text{if } r = 0 \\ 2\pi^2 a/r, & \text{if } r \neq 0 \end{cases}. \quad (146)$$

which corresponds to the blue curve in Figure 2. Finally the in-scattering function is

$$\Sigma^{in}(r_1, r_2, k, E) = \frac{M_{PZ}^2 k_B T}{\rho v_a^2 (2\pi)^3 a} G^n(r_1, r_2, k, E) I(|r_1 - r_2|). \quad (147)$$

We can see that it rapidly decreases for larger distances between grid points. As a crude approximation, one can still consider only diagonal terms with $r_1 = r_2$.

Scattering with polar optical phonons has the coupling constant

$$M_{POP}^2 = \frac{\rho e^2 \omega_0^2}{\epsilon_0} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \frac{q^2}{(q^2 + q_0^2)^2}. \quad (148)$$

where q_0 is the inverse screening length, and q_0 is the high frequency dielectric constant. The in-scattering function is

$$\begin{aligned} \Sigma^{in}(r_1, r_2, k_t, E) &= \frac{e^2 \hbar \omega_0 (n_0 + 1)}{2\epsilon_0 a} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \frac{a}{V} \sum_{q^l, q^t} \frac{q^2}{(q^2 + q_0^2)^2} \exp(iq_l(r_1 - r_2)) \\ &\times G^n(r_1, r_2, k_t + q_t, E + \hbar\omega_0) + \text{absorption} \end{aligned} \quad (149)$$

For this we need to calculate the dimensionless integral over momenta, a generalization of

$I(r) = J(r, 0)$, which is

$$J(r, q_0) = a \int_B \frac{q^2 \exp(iqr \cos \theta)}{(q^2 + q_0^2)^2} d^3 q. \quad (150)$$

We will consider only the case of no unconfined transverse dimensions and will leave other cases as homework for the reader ☺ ☺ ☺ .

Again approximating by spherically symmetric integral

$$J(r, q_0) = a \int_0^{qm} dq \frac{q^4}{(q^2 + q_0^2)^2} 4\pi \text{sinc}(qr) . \quad (151)$$

The in-scattering function is (still for the case of no transverse momenta)

$$\begin{aligned} \Sigma^{in}(r_1, r_2, E) &= \frac{e^2 \hbar \omega_0}{2\epsilon_0 a (2\pi)^3} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) J(|r_1 - r_2|, q_0) \\ &\times \left(G^n(r_1, r_2, E + \hbar \omega_0)(n_0 + 1) + G^n(r_1, r_2, E - \hbar \omega_0)n_0 \right) . \end{aligned} \quad (152)$$

This integral is more complicated and is best to evaluate numerically. The results are presented in Figure 2. It shows the off-diagonal terms can be neglected within a reasonable approximation.

This approximation gets better for stronger screening.

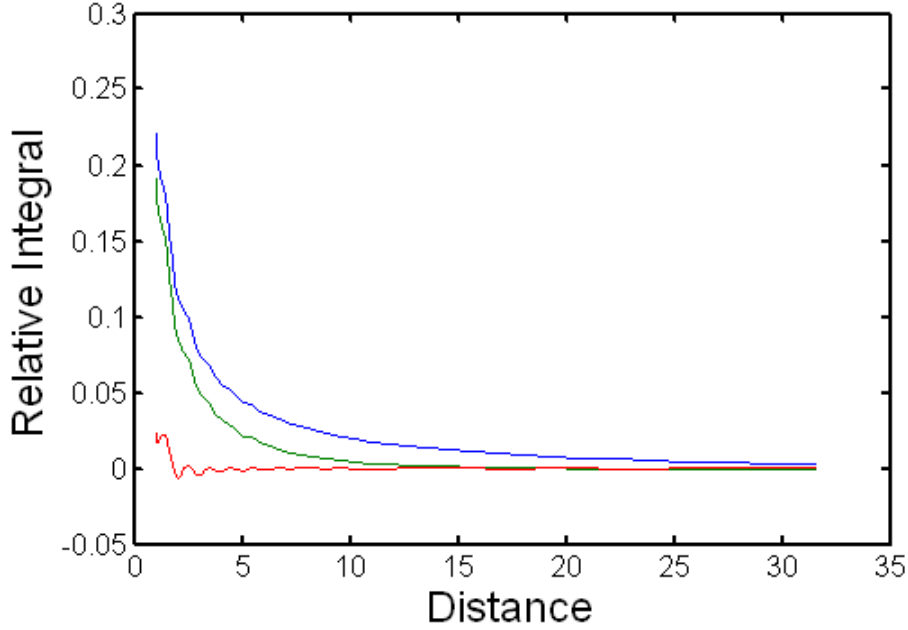


FIG 2. Relative values of the integral $J(r, q_0)$ in units of $J(0,0) = 8\pi^2$ (the value for zero distance) as a function of distance r in units of the lattice constant a for values of $q_0 = 0, 0.1, 1$ - blue, green, and red curves, respectively.

In summary, for important special cases, phonon scattering can be approximated by simple expressions such as (126) and (138), diagonal in coordinate indices, with the following coupling constants

$$K_o = \frac{\hbar D_o^2}{2\rho\omega_o a^3}. \quad (153)$$

$$K_a = \frac{D_a^2 k_B T}{\rho a^3 v_a^2}. \quad (154)$$

$$K_{PZ} = \frac{M_{PZ}^2 k_B T}{\rho v_a^2 a (2\pi)^3} I(0). \quad (155)$$

$$K_{POP} = \frac{e^2 \hbar \omega_0}{2\epsilon_0 a (2\pi)^3} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) J(0, q_0). \quad (156)$$

These expressions for the coupling constants will remain unchanged for various cases of unconfined and confined dimensions. The Green's functions have units of [1/energy], the scattering functions have the units of [energy], thus the coupling constants have the units of [energy²]. The reader is encouraged to verify it in her calculations.

Mode-space approach to confined dimensions

If the carriers are confined in one of the transverse dimensions, their electronic states are separated into modes (subbands) associated with the transverse wavefunction $\psi_n(r_t)$. We shall transform to that basis of modes according to rules

(29) and (30) and obtain a general expression

$$\begin{aligned} \Sigma^{in}(r_{1l}, r_{2l}, m, n, E) = & \sum_{r_{1t}, r_{2t}, q_l, q_t, \alpha, \beta} \psi_m^*(r_{1t}) \psi_\beta^*(r_{2t}) \psi_n(r_{2t}) \psi_\alpha(r_{1t}) \exp(iq_t(r_{1t} - r_{2t})) \\ & \times |M_q|^2 a_q^2 (n_q + 1) G^n(r_{1l}, r_{2l}, \alpha, \beta, E + \hbar\omega_q) \exp(iq_l(r_{1l} - r_{2l})) + \text{absorption} \end{aligned} \quad (157)$$

This expressions assume a simple form in the case of the scattering function diagonal in the coordinate space (as is approximately true in the four cases considered above) and of the Green's function diagonal in the mode space (i.e., neglecting correlation between electrons in different modes).

$$\begin{aligned} \Sigma^{in}(r_{ll}, r_{ll}, m, E) &= \sum_{r_i, \alpha} \psi_m^*(r_i) \psi_\alpha^*(r_i) \psi_m(r_i) \psi_\alpha(r_i) \\ &\times \sum_q |M_q|^2 a_q^2 (n_q + 1) G^n(r_{ll}, r_{ll}, \alpha, E + \hbar\omega_q) + \text{absorption} \end{aligned} \quad (158)$$

Expressing it via the constant coupling constants (as in the cases above)

$$\begin{aligned} \Sigma^{in}(r_{ll}, r_{ll}, m, E) &= K_o (n_0 + 1) \sum_\alpha G^n(r_{ll}, r_{ll}, \alpha, E + \hbar\omega_q) F(m, \alpha) \\ &+ K_o n_0 \sum_\alpha G^n(r_{ll}, r_{ll}, \alpha, E - \hbar\omega_0) F(m, \alpha) \end{aligned}, \quad (159)$$

$$\begin{aligned} \Sigma^{out}(r_{ll}, r_{ll}, m, E) &= K_o (n_0 + 1) \sum_\alpha G^p(r_{ll}, r_{ll}, \alpha, E - \hbar\omega_q) F(m, \alpha) \\ &+ K_o n_0 \sum_\alpha G^p(r_{ll}, r_{ll}, \alpha, E + \hbar\omega_0) F(m, \alpha) \end{aligned}, \quad (160)$$

where the form-factor for scattering is

$$F(m, \alpha) = \sum_{r_i} \psi_m^*(r_i) \psi_\alpha^*(r_i) \psi_m(r_i) \psi_\alpha(r_i). \quad (161)$$

In other words, the effect of the confined modes in transverse direction is accounted by summation of all possible transitions between the modes with corresponding form-factors.

Note that the form-factors even for the same mode $F(m, m)$ are not close to unity! Let us consider albeit a limited example a case of a uniform wavefunction $\psi_m(y)$ in one confined dimension. If the simulation size along this dimension is L_y , and the grid size is a_y , so that the number of intervals is $N_y = L_y / a_y$. Then the normalization implies that

$$|\psi_m(r_i)| = \frac{1}{\sqrt{N_y}}, \quad F(m, m) = \frac{1}{N_y}. \quad (162)$$

The factor of the grid size in the numerator of the form-factor would cancel with that in the denominator of the coupling constants (153)-(156), for example

$$\Sigma^{in}(r_{1l}, r_{1l}, m, E) \sim \frac{\hbar D_o^2}{2\rho\omega_0 a_x a_y a_z L_y} (n_0 + 1) \sum_{\alpha} G^n(r_{1l}, r_{1l}, \alpha, E + \hbar\omega_q) + \text{absorption} \quad (163)$$

and therefore the results do not depend on the choice of the grid size in the confined dimension.

Integration over unconfined transverse dimensions

This approximation is especially relevant to 1D and 2D transport simulators, like nanoMOS [10] and RTD. In such cases the simulation is much more efficient, if one does not have to do the calculations for all values of the unconfined transverse momentum separately. It works in the case when the Hamiltonian is a sum of the longitudinal and transverse part and does not depend explicitly on the transverse dimensions.

$$H(k_l, k_t, r_l, r_t) = H_l(k_l, r_l) + H_t(k_t) \quad (164)$$

One but not exclusive example of it is parabolic bands

$$H_l(k_l, r_l) = \frac{\hbar^2 k_l^2}{2m_l} + V(r_l), \quad H_t(k_t) = \frac{\hbar^2 k_t^2}{2m_t} = E_t \quad (165)$$

We start from the equation for the Green's function

(3). Here we separate the self-energy originating from contacts and from phonon scattering.

$$G(k_t, E) = \left[(E + i\eta^+) I - H_l - H_t - \Sigma_c(E) - \Sigma_s(E) \right]^{-1} \quad (166)$$

[Note that the self-energy does not have to be independent of the transverse momentum.] Typically, if there is no geometrical variation in the unconfined dimensions, the contact self-energy is dependent only on the barriers and band alignment in the longitudinal dimension. Upon separating the transverse and longitudinal parts

$$G(k_t, E_l + E_t) = \left[(E - E_t + i\eta^+) I - H_l - \Sigma_c(E_l) - \Sigma_s(E_l + E_t) \right]^{-1} \quad (167)$$

If we prove that the phonon self-energy can be approximated by an expression which does not have an explicit dependence on the transverse momentum, then it is possible to solve the same equation for the Green's function independent of the transverse momentum. This drastically simplifies the solution of the transport problem.

$$G(E_l) = \left[(E_l + i\eta^+) I - H_l - \Sigma_c(E_l) - \Sigma_s(E_l) \right]^{-1} \quad (168)$$

In this formulation, the Green's function depends only on the longitudinal energy and is independent of the transverse one. As for the electron and hole correlation functions, we prefer to deal with them when they are summed over the values of the transverse momentum. This way we take out of consideration the details of their behavior in the transverse dimension and focus on the transport dimension. [Here $U=3-C$ is the number of unconfined dimensions.] The summed electron and hole correlation functions are

$$\tilde{G}^n(E_l) = \frac{a^U}{V_{unc}} \sum_{kt} G^n(k_t, E_l + E_t) \quad (169)$$

$$\tilde{G}^p(E_l) = \frac{a^U}{V_{unc}} \sum_{kt} G^p(k_t, E_l + E_t) \quad (170)$$

Provided that the Green's function is independent of the transverse momentum, the summed Green's function is equal to itself

$$\tilde{G}(E_l) = \frac{a^U}{V_{unc}} \sum_{kt} G(E_l) = G(E_l). \quad (171)$$

Note that these summations are over the transverse momentum (or equivalently transverse energy) at a constant value of longitudinal energy. It is different from the frequently used summation over states with the constant total energy. Also the factors in the above two equations are dimensionless, so the summed electron and hole correlation functions still have the right units, [1/energy]. In a similar way we can introduce the summed in- and out-scattering functions

$$\tilde{\Sigma}^{in/out}(E_l) = \frac{a^U}{V_{unc}} \sum_{kt} \Sigma^{in/out}(k_t, E_l + E_t), \quad (172)$$

which are used to calculate the electron and hole correlation functions in a usual manner

$$\tilde{G}^n(E) = G \tilde{\Sigma}^{in} G^\dagger \quad (173)$$

$$\tilde{G}^p(E) = G \tilde{\Sigma}^{out} G^\dagger \quad (174)$$

The summed spectral function (in view of (171)) is determined as

$$\tilde{A}(E) = A(E) = \tilde{G}^n(E) + \tilde{G}^p(E). \quad (175)$$

The sum of electron and hole correlation functions over momenta is usually expressed via a more physically meaningful integral over momenta according to (95)

$$\tilde{G}^n = \frac{a^U}{V_{unc}} \sum_{kt} G^n = \frac{a^U}{V_{unc}} \left(\frac{L}{2\pi} \right)^U \int d^U k_t G^n = \left(\frac{a}{2\pi} \right)^U \int d^U k_t G^n. \quad (176)$$

This way, it does not include the artificial quantity of volume in the unconfined dimensions. Also the grid sizes in unconfined dimensions cancel with those in the coupling constants, like (123). Some authors introduce the integrated correlation function without this factor, which however has the units of $[J / m^U]$.

$$G_i^n = \frac{1}{V_{unc}} \sum_{kt} G^n = \left(\frac{1}{2\pi} \right)^U \int d^U k_t G^n. \quad (177)$$

Now we need to derive the expressions for the summed phonon scattering self energy and prove that they can in fact have no explicit dependence on the transverse momentum.

The case of acoustic phonons, diagonal in the coordinate space, is the simplest. The in-scattering function is proportional to the electron correlation function

$$\Sigma_s^{in}(k_t, E_l) = K_a G^n(k_t, E_l), \quad (178)$$

Then the summed in-scattering function is proportional to the summed electron correlation function and does not contain explicit dependence on the transverse momentum.

$$\tilde{\Sigma}_s^{in}(E_l) = K_a \tilde{G}^n(E_l), \quad \tilde{\Sigma}_s^{out}(E_l) = K_a \tilde{G}^p(E_l) \quad (179)$$

The self-energy is proportional to the Green's function and is thus independent of the transverse momentum. As above, it means that the summed self-energy coincides with the simple self energy

$$\tilde{\Sigma}_s(E_l) = K_a G(E_l) = \Sigma_s(E_l). \quad (180)$$

The case of optical phonons, diagonal in the coordinate space, is a bit more involved. We start with the expression (126) of the in-scattering function with unconfined dimensions

$$\begin{aligned} \Sigma^{in}(r_1, r_1, k_t, E) &= K_o (n_0 + 1) \frac{a^U}{V_{unconf}} \sum_{qt} G^n(r_1, r_1, k_t + q_t, E + \hbar\omega_0) \\ &+ K_o n_0 \frac{a^U}{V_{unconf}} \sum_{qt} G^n(r_1, r_1, k_t - q_t, E - \hbar\omega_0) \end{aligned} \quad (181)$$

By changing the variable $k_t + q_t \rightarrow k_t$, the summation can be expressed via the electron spectral functions

$$\Sigma^{in}(r_1, r_1, E_l) = K_o (n_0 + 1) \tilde{G}^n(r_1, r_1, E_l + \hbar\omega_0) + K_o n_0 \tilde{G}^n(r_1, r_1, E_l - \hbar\omega_0) \quad (182)$$

and similarly for the out-scattering function

$$\Sigma^{out}(r_1, r_1, E_l) = K_o (n_0 + 1) \tilde{G}^p(r_1, r_1, E_l - \hbar\omega_0) + K_o n_0 \tilde{G}^p(r_1, r_1, E_l + \hbar\omega_0) \quad (183)$$

The self energy must be calculated via the general expressions (7), (10), and (11). But it is obviously dependent only on the longitudinal energy. As before, the self energy coincides with the summed self-energy $\tilde{\Sigma}_s(E_l) = \Sigma_s(E_l)$. Thus in either of the above two cases, it is possible to switch from Green's functions and self energies dependent on the transverse momentum to the ones summed over the transverse momentum and no longer containing the explicit dependence on it.

Note that just like for confined transverse dimensions, the factor of the grid size in the numerator would cancel with that in the denominator of the coupling constants (153)-(156), for example

$$\Sigma^{in}(r_1, r_1, E_i) = K_o a^U (n_0 + 1) G_i^n(r_1, r_1, E_i + \hbar\omega_0) + \text{absorption} \quad (184)$$

and therefore the results do not depend on the choice of the grid size in the confined dimension.

This fact will become clearer after the consideration of a special case of the nanoMOS simulator in the section below.

Special case: nanoMOS simulator

The mathematical model of the nanoMOS simulator [10] combines all the above considered options: the transport axis is x, confined modes are considered along the z-axis, and the summation is performed over the momentum states in the unconfined y-axis. We provide the explicit expressions for this special and very important case. We also draw a connection between the quantities introduced in the present letter and those used in the simulator.

There is one difference though between our treatment on the one hand, and nanoMOS and other simulators on the other hand. We prefer to relate the electron correlation function $G^n(E)$ to one value of spin and one valley in the bandstructure as per Eqns. (12) and (18). The simulators include the factors for degenerate spin (since the materials are not ferromagnetic) and for the case of degenerate valleys directly into $G^n(E)$. We put the burden to watch for these degeneracy factors as well as for all possible scattering channels on the reader.

Next we specify the scattering functions for the nanoMOS geometry, i.e. one transport, one confined and one unconfined dimensions. We also explicitly insert the factor of valley

degeneracy to account for multiple final states for scattering. There is no spin degeneracy factor, because scattering is considered spin-independent and therefore additional spin states are not available for scattering. For the case of acoustic phonons (either deformation potential or piezoelectric) the expressions derived above result in

$$\Sigma(x, x, m, E_l) = g_v K_a \sum_n G(x, x, n, E_l) F(m, n), \quad (185)$$

where the form-factor is the sum over all grid points

$$F(m, n) = \sum_z \psi_m^*(z) \psi_n^*(z) \psi_m(z) \psi_n(z), \quad (186)$$

Similarly the in- and out-scattering functions are

$$\Sigma^{in}(x, x, m, E_l) = g_v K_a \sum_n \tilde{G}^n(x, x, n, E_l) F(m, n), \quad (187)$$

$$\Sigma^{out}(x, x, m, E_l) = g_v K_a \sum_n \tilde{G}^p(x, x, n, E_l) F(m, n), \quad (188)$$

For the case of optical phonons (either deformation potential or polar optical), the in- and out-scattering functions are

$$\begin{aligned} \Sigma^{in}(x, x, m, E_l) &= g_v K_o (n_0 + 1) \sum_n \tilde{G}^n(x, x, n, E_l + \hbar\omega_0) F(m, n) \\ &+ g_v K_o n_0 \sum_n \tilde{G}^n(x, x, n, E_l - \hbar\omega_0) F(m, n), \end{aligned} \quad (189)$$

$$\begin{aligned} \Sigma^{out}(x, x, m, E_l) &= g_v K_o (n_0 + 1) \sum_n \tilde{G}^p(x, x, n, E_l - \hbar\omega_0) F(m, n) \\ &+ g_v K_o n_0 \sum_n \tilde{G}^p(x, x, n, E_l + \hbar\omega_0) F(m, n), \end{aligned} \quad (190)$$

The self energy needs to be calculated via the Hilbert transform (10).

For this specific case of one unconfined and one confined transverse dimension, we will again draw the connection between the in/out-scattering functions and the classical scattering rates. Following the reasoning leading to Eq. (129) and (140), for one valley

$$\frac{1}{\tau_{em,n \rightarrow m}}(E_l) = \frac{1}{\hbar} K_o (n_0 + 1) A(E_l + \hbar\omega_0) F(m, n). \quad (191)$$

The formfactor is expressed in the notation of the book [2] as

$$F(m, n) = \frac{a_y}{W_{mn}}. \quad (192)$$

The difference of the above formula from [2] is that it depends on the longitudinal energy, rather than the full energy of the particle. Fortunately, in two dimensions, the density of states (42) and the spectral functions are constant. Here again we substitute the density of state (which has a factor of 2 due to spin degeneracy) instead of the spectral function according to (23). Therefore the scattering rate becomes

$$\frac{1}{\tau_{em,n \rightarrow m}}(E) = \frac{\pi D_o^2}{2\rho\omega_0 W_{mn}} (n_0 + 1) g_{2D}(E + \hbar\omega_0). \quad (193)$$

which coincides with Eq. (2.145) of the book [2]. Here again we take into account scattering only into one valley in the electron bandstructure. A very similar approach gives the following result for scattering by acoustic phonons

$$\frac{1}{\tau_{n \rightarrow m}}(E) = \frac{\pi D_a^2 k_B T}{\hbar \rho v_a^2 W_{mm}} g_{2D}(E). \quad (194)$$

which coincides with Eq. (2.144a) of the book [2].

The expressions for density and related functions can be made more explicit too. If we consider a specific subband due to confinement in the z -dimension, the 2D density in it is

$$n_{2D} = g_s g_v \frac{1}{a_x a_y L_y} \sum_{ky} \int_{-\infty}^{+\infty} \frac{G^n(E)}{2\pi} dE \quad (195)$$

The summed electron correlation function (176) turns to

$$\tilde{G}^n = \frac{a_y}{2\pi} \int dk_y G^n. \quad (196)$$

Or in other words

$$n_{2D} = g_s g_v \frac{1}{a_x a_y} \int_{-\infty}^{+\infty} \frac{\tilde{G}^n(E_l)}{2\pi} dE_l \quad (197)$$

NanoMOS treats the band structure of carriers in the effective mass approximation with mass m .

The integral over momenta can be expressed via the integral over energies using

$$dE_y = \frac{\hbar^2 k_y dk_y}{m_y}. \quad (198)$$

Then the summed electron correlation function is

$$\tilde{G}^n = \frac{a_y \sqrt{2m_y}}{2\pi\hbar} \int_0^\infty \frac{dE_y}{\sqrt{E_y}} G^n . \quad (199)$$

Also the energy can be expressed in units of the thermal energy as $\eta = \frac{E_t}{k_B T}$. Upon that substitution

$$\tilde{G}^n = \frac{a_y}{\hbar} \sqrt{\frac{m_y k_B T}{2\pi^2}} \int_0^\infty \frac{d\eta}{\sqrt{\eta}} G^n . \quad (200)$$

NanoMOS uses a different variable in place of the electron correlation function, namely

$$N_{den} = \frac{1}{\Gamma(1/2)} \int_0^\infty \frac{d\eta}{\sqrt{\eta}} G^n . \quad (201)$$

One can similarly define the quantity for the hole density function P_{den} . This definition originates from the fact that, for ballistic conduction, the electron correlation function is determined by the Fermi function $f(\eta, \nu)$ of the contacts, where $\nu = \frac{\mu}{k_B T}$

$$G^n = G \Gamma G^+ f . \quad (202)$$

The integral over transverse momenta is expressed via the Fermi integral defined as

$$F_j(\nu) = \frac{1}{\Gamma(j+1)} \int_0^\infty \eta^j f(\eta, \nu) d\eta . \quad (203)$$

and the gamma-function $\Gamma(1/2) = \sqrt{\pi}$. The nanoMOS electron correlation function is obtained by using the in-scattering function of the type of $\Sigma^{in} = G\Gamma G^+ F_{-1/2}(\nu)$. The relation between our definition of the summed electron correlation function and that used in nanoMOS is

$$\tilde{G}^n = F_y N_{den} . \quad (204)$$

The dimensionless factor converting

$$F_y = \frac{a_y}{\hbar} \sqrt{\frac{m_y k_B T}{2\pi}} . \quad (205)$$

is related to the following factor used in nanoMOS

$$N_{2d} = \frac{1}{\hbar a_x} \sqrt{\frac{m_y k_B T}{2\pi^3}} . \quad (206)$$

Then the density of electrons is

$$n_{2D} = \frac{g_s g_v}{2} N_{2d} \int_{-\infty}^{+\infty} N_{den}(E_l) dE_l \quad (207)$$

In summary, the scattering terms in nanoMOS are

$$\begin{aligned} \Sigma^{in}(r_1, r_1, E_l) = & g_v K_o (n_0 + 1) F_y \sum_n N_{den}(x, x, n, E_l + \hbar\omega_0) F(m, n) \\ & + g_v K_o n_0 F_y \sum_n N_{den}(x, x, n, E_l - \hbar\omega_0) F(m, n) , \end{aligned} \quad (208)$$

$$\begin{aligned} \Sigma^{out}(r_1, r_1, E_l) &= g_v K_o (n_0 + 1) F_y \sum_n P_{den}(x, x, n, E_l - \hbar\omega_0) F(m, n) \\ &+ g_v K_o n_0 F_y \sum_n P_{den}(x, x, n, E_l - \hbar\omega_0) F(m, n) \end{aligned} \quad , \quad (209)$$

And for acoustic scattering

$$\Sigma^{in}(x, x, m, E_l) = g_v K_a F_y \sum_n N_{den}(x, x, n, E_l) F(m, n) \quad , \quad (210)$$

$$\Sigma^{out}(x, x, m, E_l) = g_v K_a F_y \sum_n P_{den}(x, x, n, E_l) F(m, n) \quad , \quad (211)$$

$$\Sigma(x, x, m, E_l) = g_v K_a \sum_n G(x, x, n, E_l) F(m, n) \quad , \quad (212)$$

We again stress that the solution for the Green's functions in the transport direction does not depend on the choice of the grid size in the confined and the unconfined transverse directions.

This can be verified by examining the factors in the in-scattering function

$$K_o F_y F(m, n) \propto \frac{1}{a_x a_y a_z} \cdot a_y \cdot \frac{a_z}{L_z} \quad , \quad (213)$$

So, for example, the acoustic phonon in-scattering function is

$$\Sigma^{in}(x, x, m, E_l) = g_v \frac{D_a^2 k_B T}{\rho a_x a_z v_a^2 \hbar} \sqrt{\frac{m_y k_B T}{2\pi}} F(m, m) N_{den}(x, x, m, E_l) \quad , \quad (214)$$

Conclusion

This concludes our overview of the NEGF formalism for electron scattering.

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