

Report

Quantum Transport for Nanostructures



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Chapter 1

Definition of the Different Types of Green's Functions

1.1 Introduction

Nonequilibrium Green's function techniques, initiated by Schwinger and Kadanoff and Baym [9] allow ones to study the time evolution of a many-particle quantum system. Knowing the 1-particle Green's functions of a given system, one may evaluate 1-particle quantities like carrier density or current. The many-particle information about the system is cast into self-energies, parts of the equations of motion for the Green's functions. Perturbation expansion of the Green's functions is the key to approximate the self-energies.

Green's functions provide a very powerful technique for evaluating properties of many-body system both in thermodynamic equilibrium and also in nonequilibrium situations. As an introduction, equilibrium Green's functions at zero (section 1.2) and then at finite temperature (Matsubara) (section 1.3) are summarized, before the contour ordered Green's functions for nonequilibrium situations are described (section 1.4).

1.2 Equilibrium Green's Functions at Zero Temperature

In equilibrium, one needs only one Green's function to describe a given system. The time-ordered (also called causal) zero-temperature single-particle Green's function is defined [1] as

$$G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle \Psi_0 | T^c \{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \quad (1.1)$$

Here, $|\Psi_0\rangle$ is the ground state of the interacting system governed by the time-independent Hamiltonian H with $H|\Psi_0\rangle = E|\Psi_0\rangle$. H contains a non-interacting

part H_0 for which the system can be solved exactly and a more complicated part V with all the many-body effects like carrier-carrier or carrier-phonon scattering and other effects like impurity or ionized dopant scattering, interface roughness, etc. T^c is the time-ordering operator, always moving the operator with the earlier time-argument to the right.

$$T^c\{A(t)B(t')\} = \theta(t - t')A(t)B(t') + \theta(t' - t)B(t')A(t) \quad (1.2)$$

or

$$T^c\{A(t_1)B(t_2)C(t_3)\} = C(t_3)A(t_1)B(t_2) \quad (1.3)$$

if $t_3 > t_1 > t_2$. Each time two Fermion operators are interchanged, the resulting expression changes its sign, not for other operator types. The operators $\hat{\psi}_H(x, t)$ and $\hat{\psi}_H^\dagger(x', t')$ are time-dependent, i.e. defined in the Heisenberg picture (Appendix A) and evolve according to

$$\hat{\psi}_H(x, t) = e^{iHt/\hbar}\hat{\psi}(x)e^{-iHt/\hbar} \quad (1.4)$$

with $\hat{\psi}(x)$ destroying a particle at place x

$$\hat{\psi}(x) = \sum_k \phi_k(x)c_k. \quad (1.5)$$

c_k^\dagger and c_k are the usual creation and annihilation operators of a particle in state ϕ_k , respectively.

Inserting equation (1.4) into equation (1.1), the physical interpretation of the Green's functions becomes obvious

$$G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle \Psi_0 | T^c \{ e^{iHt/\hbar} \hat{\psi}(x) e^{-iH(t-t')/\hbar} \hat{\psi}^\dagger(x') e^{-iHt'/\hbar} \} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \quad (1.6)$$

If $t > t'$, the Green's function $G(x, t; x', t')$ is the probability that a particle created at time t' at place x' moves to time t and place x . This comes from the definition of $G(x, t; x', t')$: from the ground state $|\Psi_0\rangle$ at zero time, the system evolves to time t' with the factor $e^{-iHt'/\hbar}$. At this time a particle is created at place x' ($\hat{\psi}^\dagger(x')$). Then, the system continues its evolution from t' to t with the development $e^{-iH(t-t')/\hbar}$, after which the particle is destroyed at place x with the annihilation $\hat{\psi}(x)$. The system comes back to the initial ground state $|\Psi_0\rangle$ with the evolution $e^{iHt/\hbar}$. The contrary holds if $t' > t$.

To obtain $G(x, t; x', t')$, a perturbation expansion is very useful. However, the definition of the Green's function does not allow a direct solution: it involves the exact ground state $|\Psi_0\rangle$ of the system, which is one of the things to be calculated. This implies that $|\Psi_0\rangle$ must be expressed in terms of known quantities, like the eigenstates $|\phi_0\rangle$ of the non-interacting Hamiltonian H_0 . From Appendix A, in equation (A.21), one adds to the operator $V_I(t)$ a factor $\exp(-|\epsilon|t)$, which switches the interaction on and off at $t = \pm\infty$. The non-interacting ground state $|\phi_0\rangle$ is assigned to the system at $t = -\infty$ and the connection to $|\Psi_0\rangle$ is formed by the Gell-Mann

and Low theorem [10]: $|\Psi_0\rangle = S(0, -\infty)|\phi_0\rangle$. Furthermore, the system returns to its ground state $|\phi_0\rangle$ for $t = \infty$, meaning $S(\infty, -\infty)|\phi_0\rangle = e^{iL}|\phi_0\rangle$. For $G(x, t; x', t')$ it follows

$$\begin{aligned}
G(x, t; x', t') &= -\frac{i}{\hbar} \frac{\langle \phi_0 | S(-\infty, 0) T^c \{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \} S(0, -\infty) | \phi_0 \rangle}{\langle \phi_0 | S(-\infty, 0) S(0, -\infty) | \phi_0 \rangle} \\
&= -\frac{i}{\hbar} \frac{\langle \phi_0 | S(-\infty, 0) T^c \{ S(0, t) \hat{\psi}_I(x, t) S(t, 0) S(0, t') \hat{\psi}_I^\dagger(x', t') \} S(t', 0) S(0, -\infty) | \phi_0 \rangle}{\langle \phi_0 | S(-\infty, 0) S(0, -\infty) | \phi_0 \rangle} \\
&= -\frac{i}{\hbar} \frac{\langle \phi_0 | S(\infty, 0) T^c \{ S(0, t) \hat{\psi}_I(x, t) S(t, 0) S(0, t') \hat{\psi}_I^\dagger(x', t') \} S(t', 0) S(0, -\infty) | \phi_0 \rangle}{\langle \phi_0 | S(\infty, 0) S(0, -\infty) | \phi_0 \rangle} \\
&= -\frac{i}{\hbar} \frac{\langle \phi_0 | T^c \{ S(\infty, -\infty) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} | \phi_0 \rangle}{\langle \phi_0 | S(\infty, -\infty) | \phi_0 \rangle} \\
&= -\frac{i}{\hbar} \frac{\langle \phi_0 | T^c \{ \exp\left(-\frac{i}{\hbar} \int_{-\infty}^{\infty} dt_1 V_I(t_1)\right) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} | \phi_0 \rangle}{\langle \phi_0 | T^c \{ \exp\left(-\frac{i}{\hbar} \int_{-\infty}^{\infty} dt_1 V_I(t_1)\right) \} | \phi_0 \rangle}. \tag{1.7}
\end{aligned}$$

The third step was obtained by taking account of the return of the system to its ground state. This important result generates the systematic perturbation scheme for the Green's functions. The calculation proceeds by expanding the S matrix as sum of V_I products in the numerator and the denominator. A method to evaluate the resulting expectation values is needed, for example Wick's theorem (Appendix D) or the Feynman diagrams (Appendix E), which are just another way to write the results of Wick's decomposition.

Unfortunately, it is not possible to give an analytical solution for $G(x, t; x', t')$ except if the interaction perturbation V_I is set equal to zero. This gives the non-interacting or free Green's function $G_0(x - x', t - t')$ which is central for the perturbation expansions described in Appendix D and E. With the field operators given by equation (1.5) and the free particle wave function $\phi_k(x) = \frac{e^{ikx}}{\sqrt{V}}$, one gets for the free Green's function

$$\begin{aligned}
G_0(x, t; x', t') &= -\frac{i}{\hbar} \sum_{kk'} \frac{e^{i(kx - k'x')}}{V} \langle \phi_0 | T \{ c_k(t) c_{k'}^\dagger(t') \} | \phi_0 \rangle \\
&= -\frac{i}{\hbar} \sum_k \frac{e^{ik(x-x')}}{V} \langle \phi_0 | T \{ e^{iH_0 t/\hbar} c_k e^{-iH_0(t-t')/\hbar} c_k^\dagger e^{-iH_0 t'/\hbar} \} | \phi_0 \rangle \\
&= -\frac{i}{\hbar} \sum_k \frac{e^{ik(x-x')}}{V} T \{ e^{-iE_k(t-t')/\hbar} \langle \phi_0 | c_k c_k^\dagger | \phi_0 \rangle \} \\
&= G_0(x - x'; t - t'). \tag{1.8}
\end{aligned}$$

Fourier transforming both the relative coordinates $x - x'$ and $t - t'$ yields $G_0(k, \omega)$ with

$$G_0(k, \omega) = \int dx \int dt e^{-ikx} e^{i\omega t} G_0(x; t)$$

$$\begin{aligned}
&= -\frac{i}{\hbar} \sum_{k'} \int dx \frac{e^{-ix(k-k')}}{V} \left(\int_0^\infty dt e^{i(\omega-E_k/\hbar+i\eta)t} \langle \phi_0 | c_{k'} c_{k'}^\dagger | \phi_0 \rangle \right. \\
&\quad \left. - \int_{-\infty}^0 dt e^{i(\omega-E_k/\hbar-i\eta)t} \langle \phi_0 | c_{k'}^\dagger c_{k'} | \phi_0 \rangle \right) \\
&= \frac{1-f_k}{\hbar\omega-E_k+i\eta} + \frac{f_k}{\hbar\omega-E_k-i\eta}.
\end{aligned} \tag{1.9}$$

where f_k is the carrier distribution (Fermi distribution in this case because it is in equilibrium). In the zero-temperature case, the carrier distribution is a step function being 1 for energies lower than the chemical potential μ and 0 otherwise. The constant η , which tends to 0, was introduced to force the integrands to be zero at $\pm\infty$.

1.3 Equilibrium Finite Temperature Green's Functions

At finite temperature, the Green's functions are expressed in the grand canonical ensemble. The system is assumed in contact with a bath of temperature T , with whom not only heat but also particles are exchanged. At zero temperature, a bracket $\langle \cdots \rangle$ represents a ground state expectation value, but at finite temperature the system is no more in its ground state and a bracket will denote a thermodynamic average, i.e.

$$\langle O \rangle = \frac{\text{tr}(\rho O)}{\text{tr}(\rho)} = \frac{\text{tr}(e^{-\beta(H-\mu N)} O)}{\text{tr}(e^{-\beta(H-\mu N)})} = \frac{\text{tr}(e^{-\beta K} O)}{\text{tr}(e^{-\beta K})}, \tag{1.10}$$

where H is the Hamiltonian describing the system, N the particle operator, μ the chemical potential, $K = H - \mu N$, β the inverse temperature and the symbol tr stands for the trace. Then, the one-particle Green's function at finite temperature becomes

$$\begin{aligned}
G(x, t; x', t') &= -\frac{i}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T^c \{ \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') \} \right)}{\text{tr}(e^{-\beta K})} \\
&= -\frac{i}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T^c \{ e^{iKt/\hbar} \hat{\psi}(x) e^{-iK(t-t')/\hbar} \hat{\psi}^\dagger(x') e^{-iKt'/\hbar} \} \right)}{\text{tr}(e^{-\beta K})} \\
&= -\frac{i}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T^c \{ e^{iK(t-t')/\hbar} \hat{\psi}(x) e^{-iK(t-t')/\hbar} \hat{\psi}^\dagger(x') \} \right)}{\text{tr}(e^{-\beta K})}
\end{aligned} \tag{1.11}$$

The last step in equation (1.11) is due to the cyclic property of the trace and the commutation possibility between the operators $e^{-\beta(H-\mu N)}$ and $e^{-i(H-\mu N)t'/\hbar}$. The Green's function $G(x, t; x', t')$ then becomes $G(x - x', t - t')$ and the coordinate

difference $x - x'$ is Fourier transformed. This yields

$$G(k, t) = -\frac{i}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T^c \{ e^{iKt/\hbar} c_k e^{-iKt/\hbar} c_k^\dagger \} \right)}{\text{tr} (e^{-\beta K})}. \quad (1.12)$$

At this stage, it is impossible to develop a perturbation expansion as in equation (1.7) because the interaction Hamiltonian H sits in the time evolution of the field operators and in the thermal average. The Wick's decomposition described in Appendix D implies a dependence on H_0 for the thermal average and for all the field operators through the S matrix (Appendix A). This is obviously not possible for real time t and one has to define a new physical quantity, the Matsubara Green's function $\mathcal{G}(k, \tau)$.

1.3.1 Matsubara Green's Functions

To get the Matsubara Green's function $\mathcal{G}(k, \tau)$, one replaces it in equation (1.12) by τ , removes the i factor in front of G and changes the chronological time-order operator T^c to the chronological imaginary time-order operator T_τ . As consequence, one works with an imaginary time argument τ and $\mathcal{G}(k, \tau)$ is given by [1, 5]

$$\begin{aligned} \mathcal{G}(k, \tau) &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta(H-\mu N)} T_\tau \{ e^{\tau(H-\mu N)/\hbar} c_k e^{-\tau(H-\mu N)/\hbar} c_k^\dagger \} \right)}{\text{tr} (e^{-\beta(H-\mu N)})} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T_\tau \{ c_k(\tau) c_k^\dagger \} \right)}{\text{tr} (e^{-\beta K})}. \end{aligned} \quad (1.13)$$

The Green's function defined in equation (1.13) has two important properties:

- τ must be smaller than $\hbar\beta$ otherwise the convergence of the trace is not assured.
- $\mathcal{G}(k, \tau)$ is antisymmetric on the interval $-\hbar\beta < \tau < \hbar\beta$ for Fermions. This is due to the cyclic property of the trace. Considering a τ between 0 and $\hbar\beta$, one has

$$\begin{aligned} \mathcal{G}(k, \tau) &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta(H-\mu N)} c_k(\tau) c_k^\dagger \right)}{\text{tr} (e^{-\beta(H-\mu N)})} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(c_k^\dagger e^{-\beta(H-\mu N)} c_k(\tau) \right)}{\text{tr} (e^{-\beta(H-\mu N)})} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta(H-\mu N)} c_k^\dagger e^{-\beta(H-\mu N)} c_k(\tau) e^{\beta(H-\mu N)} \right)}{\text{tr} (e^{-\beta(H-\mu N)})} \\ &= -\mathcal{G}(k, \tau - \hbar\beta) \end{aligned} \quad (1.14)$$

and for $-\hbar\beta < \tau < 0$

$$\mathcal{G}(k, \tau) = -\mathcal{G}(k, \tau + \hbar\beta). \quad (1.15)$$

This last property suggests a Fourier series expansion in the strip $[-\hbar\beta, \hbar\beta]$

$$\mathcal{G}(k, \tau) = \sum_n c_n e^{-i\omega_n \tau} \quad (1.16)$$

with $\omega_n = \frac{(2n+1)\pi}{\hbar\beta}$ for Fermions and

$$c_n = \frac{1}{T} \int_{-T/2}^{T/2} d\tau \mathcal{G}(k, \tau) e^{i\omega_n \tau} = \frac{1}{2\hbar\beta} \int_{-\hbar\beta}^{\hbar\beta} d\tau \mathcal{G}(k, \tau) e^{i\omega_n \tau} = \frac{1}{\hbar\beta} \int_0^{\hbar\beta} d\tau \mathcal{G}(k, \tau) e^{i\omega_n \tau}.$$

Defining $\mathcal{G}(k, i\omega_n) = \hbar\beta c_n$ implies for the Fourier series that

$$\mathcal{G}(k, \tau) = \frac{1}{\hbar\beta} \sum_n \mathcal{G}(k, i\omega_n) e^{-i\omega_n \tau}. \quad (1.17)$$

It still remains to find a perturbation expansion for the Matsubara Green's function $\mathcal{G}(k, \tau)$. Going back to equation (1.13) and transforming the creation and annihilation operators to the pseudo-interaction picture described in Appendix B yields

$$\begin{aligned} \mathcal{G}(k, \tau) &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta K} T_\tau \{ e^{\tau K/\hbar} e^{-\tau(H_0 - \mu N)/\hbar} c_{Ik}(\tau) e^{\tau(H_0 - \mu N)/\hbar} e^{-\tau K/\hbar} c_{Ik}^\dagger \} \right)}{\text{tr} (e^{-\beta K})} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta(H_0 - \mu N)} e^{\beta(H_0 - \mu N)} e^{-\beta K} T_\tau \{ \mathcal{S}(0, \tau) c_{Ik}(\tau) \mathcal{S}(\tau, 0) c_{Ik}^\dagger \} \right)}{\text{tr} (e^{-\beta(H_0 - \mu N)} e^{\beta(H_0 - \mu N)} e^{-\beta K})} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta(H_0 - \mu N)} \mathcal{S}(\hbar\beta, 0) T_\tau \{ \mathcal{S}(0, \tau) c_{Ik}(\tau) \mathcal{S}(\tau, 0) c_{Ik}^\dagger \} \right)}{\text{tr} (e^{-\beta(H_0 - \mu N)} \mathcal{S}(\hbar\beta, 0))} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta K_0} T_\tau \{ \mathcal{S}(\hbar\beta, \tau) c_{Ik}(\tau) \mathcal{S}(\tau, 0) c_{Ik}^\dagger \} \right)}{\text{tr} (e^{-\beta K_0} \mathcal{S}(\hbar\beta, 0))} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(e^{-\beta K_0} T_\tau \{ \mathcal{S}(\hbar\beta, 0) c_{Ik}(\tau) c_{Ik}^\dagger \} \right)}{\text{tr} (e^{-\beta K_0} \mathcal{S}(\hbar\beta, 0))} \\ &= -\frac{1}{\hbar} \frac{\text{tr} \left(\rho_0 T_\tau \{ \mathcal{S}(\hbar\beta, 0) c_{Ik}(\tau) c_{Ik}^\dagger \} \right)}{\text{tr} (\rho_0 \mathcal{S}(\hbar\beta, 0))} = -\frac{1}{\hbar} \langle T_\tau \{ \mathcal{S}(\hbar\beta, 0) c_{Ik}(\tau) c_{Ik}^\dagger \} \rangle_0. \end{aligned} \quad (1.18)$$

The expression in the last line of equation (1.18) accepts the Wick's decomposition and the description by the Feynman diagrams because the thermodynamic average is made with a single particle density operator ρ_0 and \mathcal{S} , c_{Ik} and c_{Ik}^\dagger are operators represented in the interaction picture, i.e. their time evolution is governed by the one particle Hamiltonian H_0 . Therefore, the rules defined in Appendices D and E can be applied to the last line of equation (1.18). One notices that there is no imaginary i for the Matsubara Green's function $\mathcal{G}(k, \tau)$. This must be taken into account for the Feynman diagrams.

1.3.2 Advanced and Retarded Green's Functions

To make the link between imaginary and real time, two new Green's functions are introduced: the retarded G^R and the advanced G^A Fermion Green's functions, defined by (also valid in the zero temperature case)

$$\begin{aligned} G^R(x, t; x', t') &= -\frac{i}{\hbar} \theta(t - t') \langle [\hat{\psi}(x, t), \hat{\psi}^\dagger(x', t')]_+ \rangle \\ G^A(x, t; x', t') &= \frac{i}{\hbar} \theta(t' - t) \langle [\hat{\psi}(x, t), \hat{\psi}^\dagger(x', t')]_+ \rangle, \end{aligned} \quad (1.19)$$

where the brackets $\langle \dots \rangle$ mean thermodynamic average for finite temperature and ground state average for zero temperature. As usual in equilibrium, one has that the retarded and advanced Green's functions only depend on the variable differences $x - x'$ and $t - t'$. Therefore, a Fourier transformation of the space coordinates yields for G^R

$$\begin{aligned} G^R(k, t) &= -\frac{i}{\hbar} \theta(t) \langle [c_k(t), c_k^\dagger]_+ \rangle \\ &= -\frac{i}{\hbar} \theta(t) \frac{\text{tr} \left(e^{-\beta K} [e^{itK/\hbar} c_k e^{-itK/\hbar}, c_k^\dagger]_+ \right)}{\text{tr} (e^{-\beta K})} \\ &= -\frac{i}{\hbar} \theta(t) \sum_{nm} \left(\frac{\langle n | e^{-\beta K} e^{itK/\hbar} c_k e^{-itK/\hbar} | m \rangle \langle m | c_k^\dagger | n \rangle}{\text{tr} (e^{-\beta K})} + \right. \\ &\quad \left. \frac{\langle n | e^{-\beta K} c_k^\dagger | m \rangle \langle m | e^{itK/\hbar} c_k e^{-itK/\hbar} | n \rangle}{\text{tr} (e^{-\beta K})} \right) \\ &= -\frac{i}{\hbar} \theta(t) \sum_{nm} \frac{e^{-it(K_m - K_n)/\hbar} |\langle n | c_k | m \rangle|^2 (e^{-\beta K_m} + e^{-\beta K_n})}{\text{tr} (e^{-\beta K})} \end{aligned} \quad (1.20)$$

with $K|n\rangle = K_n|n\rangle$. Fourier transforming with respect to the time t yields

$$\begin{aligned} G^R(k, \omega) &= \frac{1}{\text{tr} (e^{-\beta K})} \sum_{nm} \frac{|\langle n | c_k | m \rangle|^2 (e^{-\beta K_m} + e^{-\beta K_n})}{\hbar \omega + K_n - K_m + i\delta} \\ &= [G^A(k, \omega)]^\dagger. \end{aligned} \quad (1.21)$$

Following the same procedure for the Matsubara Green's function, one obtains a similar expression

$$\mathcal{G}(k, i\omega_n) = \frac{1}{\text{tr} (e^{-\beta K})} \sum_{nm} \frac{|\langle n | c_k | m \rangle|^2 (e^{-\beta K_m} + e^{-\beta K_n})}{i\hbar\omega_n + K_n - K_m}. \quad (1.22)$$

Therefore, with knowledge of the Matsubara Green's function \mathcal{G} , for which a perturbation expansion can easily be derived, a real-time Green's function G^R can be found.

$$G^R(k, \omega) = \mathcal{G}(k, i\omega_n \rightarrow \omega + i\delta) \quad (1.23)$$

1.3.3 Fluctuation-Dissipation Theorem

To complete the set of Green's functions, two new ones are introduced, the lesser $G^<$ and the greater $G^>$ Green's functions

$$\begin{aligned} G^<(x, t; x', t') &= \frac{i}{\hbar} \langle \hat{\psi}^\dagger(x', t') \hat{\psi}(x, t) \rangle \\ G^>(x, t; x', t') &= -\frac{i}{\hbar} \langle \hat{\psi}(x, t) \hat{\psi}^\dagger(x', t') \rangle \end{aligned} \quad (1.24)$$

The chronological Green's function G (equation (1.11)), the retarded G^R and advanced G^A ones (equation (1.18)), as well as the lesser $G^<$ and greater $G^>$ Green's functions are not completely independent, but obey the relations [1]

$$G(x, t; x', t') = \theta(t - t') G^>(x, t; x', t') + \theta(t' - t) G^<(x, t; x', t') \quad (1.25)$$

$$G^{R,A}(x, t; x', t') = \pm \theta(\pm t \mp t') [G^>(x, t; x', t') - G^<(x, t; x', t')] \quad (1.26)$$

$$G^R(x, t; x', t') - G^A(x, t; x', t') = G^>(x, t; x', t') - G^<(x, t; x', t'). \quad (1.27)$$

All these properties hold both in equilibrium and in nonequilibrium case but the main feature of equilibrium theory is that all Green's functions G , $G^{<, >}$ and $G^{R,A}$ are linked via the fluctuation-dissipation theorem.

First of all, the spectral function $A(k, \omega)$ is introduced

$$A(k, \omega) = i(G^R(k, \omega) - G^A(k, \omega)) = i(G^>(k, \omega) - G^<(k, \omega)) \quad (1.28)$$

with $\int \frac{d\omega}{2\pi} A(k, \omega) = 1$. Then, with the same procedure as in the last section for the retarded Green's function G^R , one is able to show the following relation between the greater and the lesser Green's function at equilibrium

$$G^>(\omega) = -e^{\beta(\hbar\omega - \mu)} G^<(\omega) \quad (1.29)$$

and for the spectral function

$$A(k, \omega) = -i(e^{\beta(\hbar\omega - \mu)} + 1) G^<(k, \omega) \quad (1.30)$$

or

$$G^<(k, \omega) = if(\omega) A(k, \omega), \quad f(\omega) = \text{Fermi distribution.} \quad (1.31)$$

1.3.4 Relation to Observable

Observable such as particle densities or currents are directly linked to the greater and lesser Green's functions. For example

$$n(x) = -i\hbar G^<(x, t; x, t) \quad (1.32)$$

and for an homogeneous system

$$n = -\frac{i\hbar}{V} \sum_k \int \frac{d\omega}{2\pi} G^<(k, \omega) = \frac{\hbar}{V} \sum_k \int \frac{d\omega}{2\pi} A(k, \omega) f(\omega) \quad (1.33)$$

where $f(\omega)$ is the Fermi distribution in equilibrium and a distribution to determine with the Green's functions in nonequilibrium. This equation allows to give a physical interpretation to the spectral function $A(k, \omega)$ with

$$\begin{aligned} Z(\omega) &= \frac{1}{V} \sum_k \frac{A(k, \omega)}{2\pi} = \frac{i\hbar}{V} \sum_k \frac{G^R(k, \omega) - G^A(k, \omega)}{2\pi} \\ &= -\frac{\hbar}{V} \sum_k \frac{2\Im(G^R(k, \omega))}{2\pi} \end{aligned} \quad (1.34)$$

where $Z(\omega)$ is the density of states. $A(k, \omega)$ corresponds therefore to the density of state. To determine the carrier distribution in nonequilibrium, one has

$$f_{ne}(\omega) = \frac{i \sum_k G^<(k, \omega)}{2 \sum_k \Im(G^R(k, \omega))}. \quad (1.35)$$

To give an example for the spectral function $A(k, \omega)$, one considers the free retarded and advanced Green's functions:

$$\begin{aligned} G_0^R(k, \omega) &= \frac{1}{\hbar\omega - E_k + i\delta} \\ G_0^A(k, \omega) &= \frac{1}{\hbar\omega - E_k - i\delta} \end{aligned} \quad (1.36)$$

yielding for the spectral function $A(k, \omega)$

$$A(k, \omega) = 2\pi\delta(\omega - E_k/\hbar) \quad (1.37)$$

which is in agreement with the free density of states $Z(\omega) = \frac{1}{V} \sum_k \delta(\omega - E_k/\hbar)$. One will see later that the many-body effects tend to broaden the δ function present in $A(k, \omega)$.

The other observable directly related to the Green's functions is the current density. It can be expressed with the help of the lesser Green's function $G^<$

$$j(x, t) = \frac{\hbar^2}{2m} \lim_{x' \rightarrow x} (\nabla' - \nabla) G^<(x, t; x', t). \quad (1.38)$$

This simple relation will be proved in Appendix G.

1.4 Nonequilibrium Time-Loop Green's Functions

To derive the perturbation theory of the zero-temperature Green's functions, one used the fact that the system returns to its initial state for asymptotically large

times. In non-equilibrium, there is no guarantee that this occurs because the initial state at $t = -\infty$ can be very different from the final state at $t = +\infty$. Therefore, one should avoid any reference to large times in the nonequilibrium theory [1], [5] and [11].

As consequence, one has to change the way to build expectation values of an operator. If one considers the expectation value of an operator in the Heisenberg representation with respect to a state specified at t_o instead of 0 as in Appendix A, and then transforms it into the interaction representation, one has

$$\begin{aligned}
 \langle O_H(t) \rangle &= \langle S(t_o, t) O_I(t) S(t, t_o) \rangle \\
 &= \langle T^a \left\{ \exp \left(\frac{i}{\hbar} \int_{t_o}^t dt' V_I(t') \right) \right\} O_I(t) T^c \left\{ \exp \left(-\frac{i}{\hbar} \int_{t_o}^t dt' V_I(t') \right) \right\} \rangle \\
 &= \langle T^a \left\{ \exp \left(-\frac{i}{\hbar} \int_t^{t_o} dt' V_I(t') \right) \right\} O_I(t) T^c \left\{ \exp \left(-\frac{i}{\hbar} \int_{t_o}^t dt' V_I(t') \right) \right\} \rangle
 \end{aligned} \tag{1.39}$$

where $V_I(t')$ is the interaction Hamiltonian in the interaction picture and T^a the anti-chronological time-ordering operator defined in Appendix A. The perturbation evaluation of this equation may be put in a form analogous to the usual Feynman diagrams, when one joins the exponential functions from the left and right of the $O_I(t)$ operator and one introduces a time-ordering operator that recognizes whether the field operator belongs to the chronological or anti-chronological parts of the product. Accordingly, one defines the following contour, which may be imagined as lying in the complex time plane, and an operator T ordering along the contour. The

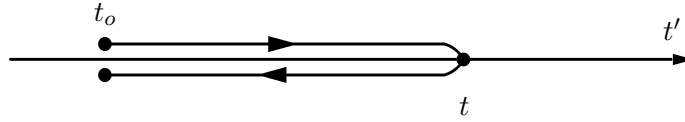


Figure 1.1: Contour along the time axis for an evaluation of the operator expectation value

T operator, reduced to the part of the contour running forward or backward in time, will become the chronological T^c or anti-chronological T^a time-ordering operator, respectively, so that the parts of the contour will be named the chronological and anti-chronological branched. Therefore, one can write equation (1.39) in the form

$$\langle O_H(t) \rangle = \langle T \left\{ \exp \left(-\frac{i}{\hbar} \oint_{t_o}^{t_o} dt' V_I(t') \right) \right\} O_I(t) \rangle, \tag{1.40}$$

where $\oint_{t_o}^{t_o}$ stands for the integral along the contour, further denoted by \int_C . By inserting extra S operators into (1.39), the contour of Figure 1.1 may be elongated, so that it would run beyond the time t . Furthermore, there is no restriction for t_o ,

which can be chosen equal to $-\infty$. This simplifies the problem as will be demonstrated later. For nonequilibrium situations, one defines a Green's function on the contour of Figure 1.1, i.e. with the time arguments from the contour,

$$G(x, t; x', t') = -\frac{i}{\hbar} \langle T \{ \hat{\psi}_{\mathcal{H}}(x, t) \hat{\psi}_{\mathcal{H}}^\dagger(x', t') \} \rangle \quad (1.41)$$

and the contour C running beyond the largest argument of the Green's function. The field operators $\hat{\psi}_{\mathcal{H}}(x, t)$ and $\hat{\psi}_{\mathcal{H}}^\dagger(x', t')$ are expressed in the Heisenberg picture with respect to the total Hamiltonian $\mathcal{H}(t)$. With the help of equation (1.24), which also holds for nonequilibrium, one can rewrite (1.41) in the form

$$G(x, t; x', t') = \theta(t, t') G^>(x, t; x', t') + \theta(t', t) G^<(x, t; x', t') \quad (1.42)$$

with the function $\theta(t, t')$ defined on a contour as:

$$\theta(t, t') = \begin{cases} 1, & \text{if } t \text{ is later on a contour than } t', \\ 0, & \text{if earlier.} \end{cases} \quad (1.43)$$

The total Hamiltonian $\mathcal{H}(t)$ of the system is given by

$$\mathcal{H}(t) = H + H^{ext}(t) = H_0 + V + H^{ext}(t), \quad (1.44)$$

where H_0 is the non-interacting part of the Hamiltonian, V contains all the interactions (carrier-carrier, carrier-phonon, impurity scattering ...) and $H^{ext}(t)$ is an external perturbation driving the system out of equilibrium

$$H^{ext}(t) = \int dx \hat{\psi}^\dagger(x) U(x, t) \hat{\psi}(x) \quad (1.45)$$

containing $U(x, t)$ the external potential.

With some algebra, one can prove that the Green's function $G(x, t; x', t')$ defined in equation (1.41) takes the following form (Appendix C) [12]

$$G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle T \{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \quad (1.46)$$

where the term $S_H^{ext}(t_0, t_0)$ with

$$S_H^{ext}(t_0, t_0) = T \left\{ \exp \left(-\frac{i}{\hbar} \int_C dt H_H^{ext}(t) \right) \right\}, \quad (1.47)$$

does not allow the application of the fluctuation-dissipation theorem. C is the contour of Figure 1.1, $\langle \dots \rangle$ is the average with the statistical operator $\rho(t_0)$ of the initial state

$$\langle \dots \rangle = \frac{\text{tr}(\rho(t_0) \dots)}{\text{tr}(\rho(t_0))} = \frac{\text{tr}(e^{-H_{initial}} \dots)}{\text{tr}(e^{-H_{initial}})}. \quad (1.48)$$

$H_{initial} = \mathcal{H}_0 + \mathcal{V}$ is a time-independent operator. It describes the equilibrium state of the system before the external perturbation $U(x, t)$ is turned on. As for the

equilibrium Green's functions, carrier interactions are present in \mathcal{V} but they are switched on adiabatically at $t = -\infty$. Therefore, it is interesting to let t_0 go toward $-\infty$, where $H_{initial} = \mathcal{H}_0$ is a 1-particle operator (first condition for the application of the Wick's theorem from Appendix D). The case where initial correlations are present, i.e. $t_0 \neq -\infty$ will be treated in Appendix H.

Neglecting the initial correlations ($t_0 = -\infty$) and rewriting equation (1.46) yields an expression for the nonequilibrium Green's function $G(x, t; x', t')$ admitting the Wick's decomposition and the Feynman diagrams

$$G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle T \left\{ S_{H_0}^{ext}(t_0, t_0) S_{H_0}^V(t_0, t_0) \hat{\psi}_{H_0}(x, t) \hat{\psi}_{H_0}^\dagger(x', t') \right\} \rangle_0}{\langle S_{H_0}^{ext}(t_0, t_0) S_{H_0}^V(t_0, t_0) \rangle_0} \quad (1.49)$$

where $t_0 = -\infty$ and

$$\begin{aligned} S_{H_0}^{ext}(t_0, t_0) &= T \left\{ \exp \left(-\frac{i}{\hbar} \int_C dt H_{H_0}^{ext}(t) \right) \right\} \\ S_{H_0}^V(t_0, t_0) &= T \left\{ \exp \left(-\frac{i}{\hbar} \int_C dt V_{H_0}(t) \right) \right\}. \end{aligned} \quad (1.50)$$

Quantum transport at finite temperature can only be described by the nonequilibrium Green's functions. The zero temperature and Matsubara Green's functions are well suited for equilibrium situations, like reservoirs responsible for the carrier injection in the device.

Chapter 2

Nonequilibrium Green's Functions

2.1 Introduction

In the previous chapter, the different types of Green's functions were introduced and it was highlighted that quantum transport occurs only in the frame of nonequilibrium Green's functions. In this chapter, the main equations governing the behavior of nonequilibrium Green's functions are presented as well as the derivation of two important physical quantities resulting from their solution, the carrier density and the current density.

2.2 Nonequilibrium Equations of Motion

Apart from the Feynman diagrams and the Wick's decomposition, another way to calculate the time evolution of nonequilibrium Green's functions $G(x, t; x', t')$ consists in deriving its equations of motion, one for the time t and another for t' . For that purpose, the time-independent part $H = H_0 + V$ of the total Hamiltonian \mathcal{H} is required. $H^{ext}(t)$ will be included through the time evolution operator $S_H^{ext}(t_0, t_0)$ of equation (1.46). H contains only the carrier-carrier interactions here, carrier-phonon scattering will be treated in Appendix F. This yields for H

$$\begin{aligned} H &= H_0 + V \\ &= \int dx \, \hat{\psi}^\dagger(x) \left(-\frac{\hbar^2 \nabla_x^2}{2m} \right) \hat{\psi}(x) \\ &\quad + \frac{1}{2} \int dx \int dy \, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) V(x-y) \hat{\psi}(y) \hat{\psi}(x). \end{aligned} \quad (2.1)$$

To derive the equations of motion for the nonequilibrium Green's function, one has to evaluate $\frac{d}{dt}G(x, t; x', t')$ or $\frac{d}{dt'}G(x, t; x', t')$ with $G(x, t; x', t')$ defined as in equations (1.41) and (1.46). First of all, this requires the definition of some mathematical

expressions: $1 = (x_1, t_1)$, $V(1-2) = V(x_1 - x_2)\delta(t_1 - t_2)$, $\int_C d1 = \int_C dt_1 \int dx_1$, where the time is integrated along a contour C such as the one of Figure 1.1,

$$\frac{d}{dt}\theta(t, t') = \delta(t, t') = \begin{cases} \frac{d}{dt}\theta(t - t') = \delta(t - t'), & \text{on the chronological branch of } C \\ \frac{d}{dt}\theta(t' - t) = -\delta(t - t'), & \text{on the anti-chronological one} \end{cases}$$

and $\delta(11') = \delta(t_1, t'_1)\delta(x_1 - x'_1)$. Furthermore, the following equation has to be evaluated in order to obtain $\frac{d}{dt}G(x, t; x', t')$:

$$\begin{aligned} \frac{d}{dt}T\left\{\hat{\psi}_{\mathcal{H}}(x, t)\hat{\psi}_{\mathcal{H}}^\dagger(x', t')\right\} &= T\left\{\frac{d}{dt}\hat{\psi}_{\mathcal{H}}(x, t)\hat{\psi}_{\mathcal{H}}^\dagger(x', t')\right\} + \delta(t, t')\left[\hat{\psi}_{\mathcal{H}}(x, t)\hat{\psi}_{\mathcal{H}}^\dagger(x', t)\right]_+ \\ &= T\left\{\frac{d}{dt}\hat{\psi}_{\mathcal{H}}(x, t)\hat{\psi}_{\mathcal{H}}^\dagger(x', t')\right\} + \delta(t, t')\delta(x - x'), \end{aligned}$$

to take into account the time-ordering operator T ,

$$\begin{aligned} i\hbar T\left\{\frac{d}{dt}\left(S_H^{ext}(t_0, t_0)\hat{\psi}_H(x, t)\hat{\psi}_H^\dagger(x', t')\right)\right\} &= i\hbar T\left\{\frac{d}{dt}\left(S_H^{ext}(t_0, t)\hat{\psi}_H(x, t)S_H^{ext}(t, t_0)\dots\right)\right\} \\ &= T\left\{S_H^{ext}(t_0, t_0)i\hbar\frac{d}{dt}\hat{\psi}_H(x, t)\hat{\psi}_H^\dagger(x', t')\right\} \\ &\quad + T\left\{S_H^{ext}(t_0, t_0)U(x, t)\hat{\psi}_H(x, t)\hat{\psi}_H^\dagger(x', t')\right\}, \end{aligned}$$

to look after the time evolution S_H^{ext} , and

$$\begin{aligned} i\hbar\frac{d}{dt}\hat{\psi}_H(x, t) &= \left[\hat{\psi}_H(x, t), H_H(t)\right] \\ &= -\frac{\hbar^2\nabla_x^2}{2m}\hat{\psi}_H(x, t) + \int dy V(x - y)\hat{\psi}_H^\dagger(y, t)\hat{\psi}_H(y, t)\hat{\psi}_H(x, t) \end{aligned}$$

for the operator derivative (Heisenberg equation of motion).

2.2.1 Dyson Equations

With the previous considerations, the equation of motion for $G(x_1, t_1; x'_1, t'_1) = G(11')$ relative to t_1 becomes

$$\left(i\hbar\frac{d}{dt_1} + \frac{\hbar^2\nabla_1^2}{2m} - U(1)\right)G(11') = \delta(11') - i\hbar\int_C d3 V(1-3)G^{(2)}(13^-1'3^+) \quad (2.2)$$

and relative to t'_1

$$\left(-i\hbar\frac{d}{dt'_1} + \frac{\hbar^2\nabla_{1'}^2}{2m} - U(1')\right)G(11') = \delta(11') - i\hbar\int_C d3 V(1'-3)G^{(2)}(13^-1'3^+) \quad (2.3)$$

where the 2-particle Green's function $G^{(2)}(131'3')$ is defined by

$$G^{(2)}(131'3') = \left(-\frac{i}{\hbar}\right)^2 \frac{\langle T \{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(1) \hat{\psi}_H(3) \hat{\psi}_H^\dagger(3') \hat{\psi}_H^\dagger(1') \} \rangle_0}{\langle S_H^{ext}(t_0, t_0) \rangle_0}. \quad (2.4)$$

The self-energy $\Sigma^{tot}(12)$ can be introduced into equation (2.2) and (2.3) via variational derivation as described in Appendix F. This gives for the equations of motion the two following fundamental expressions

$$\left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1)\right) G(11') = \delta(11') + \int_C d3 \Sigma^{tot}(13) G(31') \quad (2.5)$$

$$\left(-i\hbar \frac{d}{dt_{1'}} + \frac{\hbar^2 \nabla_{1'}^2}{2m} - U(1')\right) G(11') = \delta(11') + \int_C d3 G(13) \Sigma^{tot}(31'). \quad (2.6)$$

They correspond to the Dyson equations

$$G(11') = G_0(11') + \int_C d2 \int_C d3 G_0(12) \Sigma^{tot}(23) G(31') \quad (2.7)$$

$$G(11') = G_0(11') + \int_C d2 \int_C d3 G(12) \Sigma^{tot}(23) G_0(31') \quad (2.8)$$

where $G_0(12)$ is the free or non-interacting nonequilibrium Green's function and $G_0^{-1}(12)$ its inverse, defined by

$$G_0(12) = \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1)\right)^{-1} \delta(12) \quad (2.9)$$

$$G_0^{-1}(12) = \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1)\right) \delta(12). \quad (2.10)$$

This gives the following relations

$$\int_C d2 G_0^{-1}(12) G_0(21') = \delta(11') \quad (2.11)$$

$$\int_C d2 G_0^{-1}(12) G(21') = \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1)\right) G(11'). \quad (2.12)$$

The nonequilibrium equations of motion contain integrals over a time-loop \int_C which have to be divided into time-ordered integrals. This occurs by considering the equations of motion of all the previously defined types of Green's functions, $G^{R,A}$ and $G^{<,>}$ among other.

2.3 Langreth Theorem [1]

In the equations of motion (2.5) and (2.6), one encounters terms with the structure $C = AB$, or, explicitly,

$$C(t_1, t'_1) = \int_{C_1} d\tau A(t_1, \tau) B(\tau, t'_1), \quad (2.13)$$

where C_1 is the contour of figure 1.1. To evaluate (2.13), one assumes for definiteness that t_1 is on the first half of C_1 (chronological branch) and t_2 on the second, as shown on Figure 2.1. With the definition of C analog to equation (1.42)

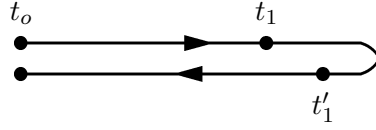


Figure 2.1: Contour C_1 along the time axis for an evaluation of the operator expectation value $C = AB$

$$C(t_1, t'_1) = \theta(t_1, t'_1) C^>(t_1, t'_1) + \theta(t'_1, t_1) C^<(t_1, t'_1), \quad (2.14)$$

one immediately sees that the above placement of t_1 and t'_1 leads to the definition of the lesser function $C^<(t_1, t'_1)$. As stated before, the contour C_1 of figure 2.1 can be elongated and/or deformed to give the sum of contours C_2 and C'_2 from figure 2.2. Thus, equation (2.13) becomes

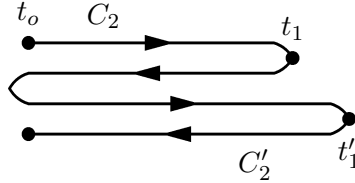


Figure 2.2: Deformation of contour C_1 into contour C_2 and C'_2 for the evaluation of $C = AB$

$$C^<(t_1, t'_1) = \int_{C_2} d\tau A(t_1, \tau) B^<(\tau, t'_1) + \int_{C'_2} d\tau A^<(t_1, \tau) B(\tau, t'_1). \quad (2.15)$$

$B(\tau, t'_1)$ is equal to $B^<(\tau, t'_1)$ if τ is on contour C_2 because t'_1 is always later than τ in this case. The same proof holds for $A^<(t_1, \tau)$ with τ on C'_2 . Now the first term in equation (2.15) is considered and the integral is divided into two parts

$$\begin{aligned} \int_{C_2} d\tau A(t_1, \tau) B^<(\tau, t'_1) &= \int_{-\infty}^{t_1} dt A^>(t_1, t) B^<(\tau, t'_1) + \int_{t_1}^{-\infty} dt A^<(t_1, t) B^<(\tau, t'_1) \\ &= \int_{-\infty}^{t_1} dt (A^>(t_1, t) - A^<(t_1, t)) B^<(\tau, t'_1) \\ &= \int_{-\infty}^{\infty} dt A^R(t_1, t) B^<(\tau, t'_1). \end{aligned} \quad (2.16)$$

In the first line, $A(t_1, t)$ is equal to $A^>(t_1, t)$ if $-\infty < t < t_1$ because t_1 is later than t for this particular case. The same reasoning can be applied to find $A^<(t_1, t)$ when $t_1 > t > -\infty$. The last line is obtained by recalling the definition of the retarded functions from equation (1.26). A similar analysis can be applied to the second term of equation (2.15) involving contour C'_2 . Putting the two terms together, one finds Langreth's first result

$$C^<(t_1, t'_1) = \int_{-\infty}^{\infty} dt (A^R(t_1, t)B^<(t, t'_1) + A^<(t_1, t)B^A(t, t'_1)) \quad (2.17)$$

and therefore in compact notation $\boxed{C^< = A^R B^< + A^< B^A}$. The same result applies to the "greater" function $C^>$, one just needs to replace all the $<$'s by $>$'s. The retarded and advanced functions C^R and C^A , respectively are also of central importance and are obtained from equation (1.26). For example, one has for $C^R(t_1, t'_1)$

$$\begin{aligned} C^R(t_1, t'_1) &= \theta(t_1 - t'_1) (C^>(t_1, t'_1) - C^<(t_1, t'_1)) \\ &= \theta(t_1 - t'_1) \int_{-\infty}^{\infty} dt (A^R [B^> - B^<] + [A^> - A^<] B^A) \\ &= \theta(t_1 - t'_1) \left[\int_{-\infty}^{t_1} dt (A^> - A^<)(B^> - B^<) \right. \\ &\quad \left. + \int_{-\infty}^{t'_1} dt (A^> - A^<)(B^< - B^>) \right] \\ &= \int_{t'_1}^{t_1} dt (A^> - A^<)(B^> - B^<) \\ &= \int_{t'_1}^{t_1} dt A^R(t_1, t)B^R(t, t'_1). \end{aligned} \quad (2.18)$$

In the compact form, this relation is expressed as $\boxed{C^R = A^R B^R}$ and for the advanced function $C^A = A^A B^A$.

In the Dyson equations (2.7) and (2.8), products of three functions $D = ABC$ appear with

$$\begin{aligned} D(t_1, t'_1) &= \int_{C_1} d\tau_1 \int_{C_1} d\tau_2 A(t_1, \tau_1)B(\tau_1, \tau_2)C(\tau_2, t'_1) \\ &= \int_{C_1} d\tau_1 A(t_1, \tau_1)B'(\tau_1, t'_1) \end{aligned} \quad (2.19)$$

and

$$B'(\tau_1, t'_1) = \int_{C_1} d\tau_2 B(\tau_1, \tau_2)C(\tau_2, t'_1). \quad (2.20)$$

Hence, to get $D^<$ for example, equations (2.17) and (2.18) can be directly applied and one finds in the compact notation

$$D^< = A^R B^R C^< + A^R B^< C^A + A^< B^A C^A. \quad (2.21)$$

Other structures are of great interest in order to evaluate the self energies

$$\begin{aligned} C(t, t') &= A(t, t')B(t, t') \\ D(t, t') &= A(t, t')B(t', t) \end{aligned}$$

where t and t' are contour variables. It is obvious that

$$\begin{aligned} C^<(t, t') &= A^<(t, t')B^<(t, t') \\ D^<(t, t') &= A^<(t, t')B^>(t', t) \end{aligned}$$

and a little more complicated for C^R , C^A , D^R and D^A

$$\begin{aligned} C^R(t, t') &= \theta(t - t') (C^>(t, t') - C^<(t, t')) \\ &= \theta(t - t') (A^>(t, t')B^>(t, t') - A^<(t, t')B^<(t, t')) \\ &= \theta(t - t') (A^>(t, t')B^>(t, t') - A^<(t, t')B^>(t, t') \\ &\quad + A^<(t, t')B^>(t, t') - A^<(t, t')B^<(t, t')) \\ &= A^R(t, t')B^>(t, t') + A^<(t, t')B^R(t, t') \\ &= A^R(t, t')B^>(t, t') - A^R(t, t')B^<(t, t') + \\ &\quad A^R(t, t')B^<(t, t') + A^<(t, t')B^R(t, t') \\ &= A^R(t, t')B^R(t, t') + A^R(t, t')B^<(t, t') + A^<(t, t')B^R(t, t') \\ C^A(t, t') &= A^A(t, t')B^A(t, t') + A^A(t, t')B^>(t, t') + A^>(t, t')B^A(t, t') \\ &= -A^A(t, t')B^A(t, t') + A^A(t, t')B^<(t, t') + A^<(t, t')B^A(t, t'), \\ D^R(t, t') &= A^R(t, t')B^<(t', t) + A^<(t, t')B^A(t', t), \\ D^A(t, t') &= A^A(t, t')B^>(t', t) + A^>(t, t')B^R(t', t). \end{aligned} \tag{2.22}$$

All these relations will be useful to compute the time evolution and the self-energies of the Green's functions.

2.4 Eigenfunction Expansion

The Green's functions $G(11')$ depend on the continuous space variables \mathbf{r} and \mathbf{r}' . To solve a real problem in 1-, 2-, or 3-D, it is better to work with discretized Green's functions $G_{nm}(tt')$. In this section, one will give an example for a 1-D structure with transport in the z -direction and homogeneous potential in the x - and y -transverse directions (the procedure is straightforward for 2- and 3-D). For that purpose, one recalls equation (1.5), where the creation and annihilation operators $\hat{\psi}^\dagger(x', t')$ and $\hat{\psi}(x, t)$ are expanded into a series of eigenfunctions. Thus, $G(11')$ can be written as [2, 13]

$$G(11') = \sum_{n_1, m_1} \sum_{\mathbf{k}', \mathbf{k}''} \phi_{n_1, \mathbf{k}'}(\mathbf{r}) \cdot G_{n_1 m_1}(\mathbf{k}' \mathbf{k}''; tt') \cdot \phi_{m_1, \mathbf{k}''}^*(\mathbf{r}'). \tag{2.23}$$

For homogeneity in the x - and y - directions and confinement in the z -one, one can factorize the wave functions ϕ as

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{A}} e^{i\mathbf{k}_t \cdot \mathbf{r}_t} \phi_{\mathbf{k}_t}(z), \tag{2.24}$$

where A is the xy surface, $\mathbf{k}_t = (k_x, k_y)$, and $\mathbf{r}_t = (x, y)$. Furthermore, because of the homogeneity in the x - and y - directions, the Green's function $G(11')$ depends only on the difference $\mathbf{r}_t - \mathbf{r}'_t$ and, therefore, $\mathbf{k}'_t = \mathbf{k}''_t$. This gives

$$G(11') = \frac{1}{A} \sum_{n_1, m_1} \sum_{\mathbf{k}'_t} \phi_{n_1, \mathbf{k}'_t}(z) \cdot G_{n_1 m_1}(\mathbf{k}'_t; tt') \cdot \phi_{m_1, \mathbf{k}'_t}^*(z') \cdot e^{i\mathbf{k}'_t \cdot (\mathbf{r}_t - \mathbf{r}'_t)}. \quad (2.25)$$

The wave functions ϕ should be very localized functions, for example orbital functions around one lattice point [4, 14] or Wannier functions localized on one quantum well [3] or on one period of a superlattice [15]. In accordance with the orthogonality of the basis functions, one establishes the inverse transformation

$$G_{nm}(\mathbf{k}_t; tt') = \int d(\mathbf{r}_t - \mathbf{r}'_t) \int dz \int dz' \phi_{n, \mathbf{k}_t}^*(z) \cdot G(11') \cdot \phi_{m, \mathbf{k}_t}(z') \cdot e^{-i\mathbf{k}_t \cdot (\mathbf{r}_t - \mathbf{r}'_t)}. \quad (2.26)$$

The same relations are also available for the self-energies $\Sigma(11')$

$$\Sigma(11') = \frac{1}{A} \sum_{n_1, m_1} \sum_{\mathbf{k}'_t} \phi_{n_1, \mathbf{k}'_t}(z) \cdot \Sigma_{n_1 m_1}(\mathbf{k}'_t; tt') \cdot \phi_{m_1, \mathbf{k}'_t}^*(z') \cdot e^{i\mathbf{k}'_t \cdot (\mathbf{r}_t - \mathbf{r}'_t)} \quad (2.27)$$

$$\Sigma_{nm}(\mathbf{k}_t; tt') = \int d(\mathbf{r}_t - \mathbf{r}'_t) \int dz \int dz' \phi_{n, \mathbf{k}_t}^*(z) \cdot \Sigma(11') \cdot \phi_{m, \mathbf{k}_t}(z') \cdot e^{-i\mathbf{k}_t \cdot (\mathbf{r}_t - \mathbf{r}'_t)}. \quad (2.28)$$

Recalling the equations of motion for the Green's functions (2.5) and (2.6), one finds therefore

$$i\hbar \frac{d}{dt} G_{nm}(\mathbf{k}_t; tt') - \sum_l h_{nl} G_{lm}(\mathbf{k}_t; tt') = \delta_{nm}(tt') + \sum_l \int_C dt_1 \Sigma_{nl}(\mathbf{k}_t; tt_1) G_{lm}(\mathbf{k}_t; t_1 t')$$

and

$$-i\hbar \frac{d}{dt'} G_{nm}(\mathbf{k}_t; tt') - \sum_l h_{ml}^* G_{nl}(\mathbf{k}_t; tt') = \delta_{nm}(tt') + \sum_l \int_C dt_1 G_{nl}(\mathbf{k}_t; tt_1) \Sigma_{lm}(\mathbf{k}_t; t_1 t')$$

where $h_{nm} = \int d\mathbf{r} \phi_n^*(\mathbf{r}) H_0(\mathbf{r}) \phi_m(\mathbf{r})$ and $h_{ml}^* = h_{lm}$, because the Hamiltonian is hermitian.

To conclude this section, one will give a small calculation example for $\Sigma_{lm}(\mathbf{k}_t; tt_1)$. The starting point is equation (F.23)

$$\Sigma(11') = i\hbar W(1'1)G(11'). \quad (2.29)$$

With the help of equation (2.28), one gets

$$\Sigma_{nm}(\mathbf{k}_t; tt') = i\hbar \int d(\mathbf{r}_t - \mathbf{r}'_t) \int dz \int dz' \phi_{n, \mathbf{k}_t}^*(z) \cdot W(1'1) \cdot G(11') \cdot \phi_{m, \mathbf{k}_t}(z') \cdot e^{-i\mathbf{k}_t \cdot (\mathbf{r}_t - \mathbf{r}'_t)}.$$

Expanding $G(11')$ in this equation yields

$$\begin{aligned}\Sigma_{nm}(\mathbf{k}_t; tt') &= \frac{i\hbar}{A} \sum_{n_1, m_1} \sum_{\mathbf{k}'_t} \int d(\mathbf{r}_t - \mathbf{r}'_t) \int dz \int dz' G_{n_1 m_1}(\mathbf{k}'_t; tt') \\ &\quad \times \phi_{n, \mathbf{k}_t}^*(z) \phi_{m, \mathbf{k}_t}(z') \cdot W(1'1) \cdot \phi_{n_1, \mathbf{k}'_t}(z) \phi_{m_1, \mathbf{k}'_t}^*(z') e^{-i(\mathbf{k}'_t - \mathbf{k}_t) \cdot (\mathbf{r}'_t - \mathbf{r}_t)} \\ &= i\hbar \sum_{n_1, m_1} \sum_{\mathbf{k}'_t} W_{nm n_1 m_1}(\mathbf{k}'_t - \mathbf{k}_t; t't) G_{n_1 m_1}(\mathbf{k}'_t; tt').\end{aligned}$$

The same procedure must be applied to obtain the discrete self-energies for electron-phonon or other interactions.

2.5 Closed Set of Equations

The carrier density and the current are two of the most important physical quantities one is looking for in a device simulation. As seen in section 1.3.4 and for nonequilibrium in section 2.7, to get the carrier $n(x, t)$ and the current $J(x, t)$ densities, one needs the lesser Green's function $G^<(x, t; x', t')$, for which the equation of motion must be solved. This is only possible, because the self-energy $\Sigma(12)$ has the same symmetry properties as the Green's function $G(12)$. This result was already used by Craig in [16] and the proof is given by Danielewicz in [11], yielding

$$\Sigma(12) = \Sigma^\delta(12) + \theta(t_1, t_2) \Sigma^>(12) + \theta(t_2, t_1) \Sigma^<(12), \quad (2.30)$$

$$\Sigma^R(12) = \Sigma^\delta(12) + \theta(t_1 - t_2) (\Sigma^>(12) - \Sigma^<(12)), \quad (2.31)$$

$$\Sigma^A(12) = \Sigma^\delta(12) - \theta(t_2 - t_1) (\Sigma^>(12) - \Sigma^<(12)), \quad (2.32)$$

$$\Sigma^R(12) - \Sigma^A(12) = \Sigma^>(12) - \Sigma^<(12) \quad (2.33)$$

with $\Sigma^\delta(12)$, defined in equation (F.26), being a singular part of $\Sigma(12)$ on the contour shown in figure 1.1.

As consequence, with Langreth theorem of section 2.3 and the eigenfunction expansion of section 2.4, one obtains

$$\begin{aligned}i\hbar \frac{d}{dt} G_{nm}^<(\mathbf{k}_t; tt') - \sum_l h_{nl} G_{lm}^<(\mathbf{k}_t; tt') &= \sum_l \int_{t_0}^{\infty} dt_1 \Sigma_{nl}^R(\mathbf{k}_t; tt_1) G_{lm}^<(\mathbf{k}_t; t_1 t') \\ &\quad + \sum_l \int_{t_0}^{\infty} dt_1 \Sigma_{nl}^<(\mathbf{k}_t; tt_1) G_{lm}^A(\mathbf{k}_t; t_1 t')\end{aligned} \quad (2.34)$$

and/or

$$\begin{aligned}
 -i\hbar \frac{d}{dt'} G_{nm}^<(\mathbf{k}_t; tt') - \sum_l G_{nl}^<(\mathbf{k}_t; tt') h_{lm} &= \sum_l \int_{t_0}^{\infty} dt_1 G_{nl}^R(\mathbf{k}_t; tt_1) \Sigma_{lm}^<(\mathbf{k}_t; t_1 t') \\
 &+ \sum_l \int_{t_0}^{\infty} dt_1 G_{nl}^<(\mathbf{k}_t; tt_1) \Sigma_{lm}^A(\mathbf{k}_t; t_1 t').
 \end{aligned} \tag{2.35}$$

To solve one of these equations, one needs different forms of the self-energy ($\Sigma^<$ and $\Sigma^{R,A}$), as well as the retarded and the advanced form of the Green's function $G^{R,A}$. Therefore, an equation of motion must be solved for them, according to 2.18

$$i\hbar \frac{d}{dt} G_{nm}^R(\mathbf{k}_t; tt') - \sum_l h_{nl} G_{lm}^R(\mathbf{k}_t; tt') = \delta_{nm}(tt') + \sum_l \int_{t_0}^{\infty} dt_1 \Sigma_{nl}^R(\mathbf{k}_t; tt_1) G_{lm}^R(\mathbf{k}_t; t_1 t')$$

or

$$-i\hbar \frac{d}{dt'} G_{nm}^R(\mathbf{k}_t; tt') - \sum_l G_{nl}^R(\mathbf{k}_t; tt') h_{lm} = \delta_{nm}(tt') + \sum_l \int_{t_0}^{\infty} dt_1 G_{nl}^R(\mathbf{k}_t; tt_1) \Sigma_{lm}^R(\mathbf{k}_t; t_1 t').$$

The equations for G^A are obtained by replacing the R 's by A 's. One can rewrite them in a compact form

$$\begin{aligned}
 \delta_{nm}(tt') &= \sum_l \int_{t_0}^{\infty} dt_1 \left(i\hbar \delta_{ln}(t_1 t) \frac{d}{dt_1} - h_{nl} \delta(t_1 t) - \Sigma_{nl}^R(\mathbf{k}_t; tt_1) \right) G_{lm}^R(\mathbf{k}_t; t_1 t') \\
 &= \sum_l \int_{t_0}^{\infty} dt_1 [G_{nl}^R(\mathbf{k}_t; tt_1)]^{-1} G_{lm}^R(\mathbf{k}_t; t_1 t').
 \end{aligned} \tag{2.36}$$

Relation 2.36 can be used to simplify the equation of motion for the lesser Green's function $G^<$

$$\sum_l \int_{t_0}^{\infty} dt_1 [G_{nl}^R(\mathbf{k}_t; t' t_1)]^{-1} G_{lm}^<(\mathbf{k}_t; t_1 t'') = \sum_l \int_{t_0}^{\infty} dt_1 \Sigma_{nl}^<(\mathbf{k}_t; t' t_1) G_{lm}^A(\mathbf{k}_t; t_1 t'').$$

Multiplying each side of the equation by $G_{pn}^R(\mathbf{k}_t; tt')$, summing over n , and integrating over t' yields

$$\begin{aligned}
 \sum_{l,n} \int_{t_0}^{\infty} dt_1 \int_{t_0}^{\infty} dt' G_{pn}^R(\mathbf{k}_t; tt') [G_{nl}^R(\mathbf{k}_t; t' t_1)]^{-1} G_{lm}^<(\mathbf{k}_t; t_1 t'') &= \sum_l \int_{t_0}^{\infty} dt_1 \delta_{pl}(tt_1) G_{lm}^<(\mathbf{k}_t; t_1 t'') \\
 &= G_{pm}^<(\mathbf{k}_t; tt'')
 \end{aligned}$$

and therefore

$$G_{nm}^<(\mathbf{k}_t; tt') = \sum_{l,v} \int_{t_0}^{\infty} dt_1 \int_{t_0}^{\infty} dt_2 G_{nl}^R(\mathbf{k}_t; tt_1) \Sigma_{lv}^<(\mathbf{k}_t; t_1 t_2) G_{vm}^A(\mathbf{k}_t; t_2 t'). \tag{2.37}$$

This is the central equation for the lesser Green's function, but there is still a coupling between $G^<$ and $G^{R,A}$.

2.5.1 Non-Interacting Green's Functions

In case of a non-interacting system, the solution of the Green's functions can be found from their definition. As example, one considers $G_{0nm}^<(k; t_1 t_2)$

$$G_{0nm}^<(k; t_1 t_2) = \frac{i}{\hbar} \langle c_{k,m}^\dagger(t_2) c_{k,n}(t_1) \rangle, \quad (2.38)$$

where the creation $c_k^\dagger(t)$ and annihilation $c_k(t)$ operators are defined with respect to the non-interacting Hamiltonian H_0

$$\begin{aligned} c_k^\dagger(t) &= e^{iH_0 t/\hbar} c_k^\dagger e^{-iH_0 t/\hbar} \\ c_k(t) &= e^{iH_0 t/\hbar} c_k e^{-iH_0 t/\hbar}. \end{aligned} \quad (2.39)$$

As consequence, one obtains for the lesser Green's function

$$G_{0nm}^<(k; t_1 t_2) = \frac{i}{\hbar} e^{iE_m t_2/\hbar} e^{-iE_n t_1/\hbar} \langle c_{k,m}^\dagger c_{k,n} \rangle. \quad (2.40)$$

The same procedure can be applied to the greater non-interacting Green's functions leading to a similar result

$$G_{0nm}^>(k; t_1 t_2) = -\frac{i}{\hbar} e^{iE_m t_2/\hbar} e^{-iE_n t_1/\hbar} \langle c_{k,n} c_{k,m}^\dagger \rangle. \quad (2.41)$$

Using equations (2.40) and (2.41) as well as the definition of the retarded and advanced Green's functions (1.26), one obtains the non-interacting expression for G^R and G^A

$$\begin{aligned} G_{0nm}^R(k; t_1 t_2) &= \theta(t_1 - t_2) (G_{0nm}^>(k; t_1 t_2) - G_{0nm}^<(k; t_1 t_2)) \\ &= -\frac{i}{\hbar} \theta(t_1 - t_2) e^{iE_m t_2/\hbar} e^{-iE_n t_1/\hbar} \langle [c_{k,n}, c_{k,m}^\dagger]_+ \rangle \\ &= -\frac{i}{\hbar} \theta(t_1 - t_2) e^{iE_m t_2/\hbar} e^{-iE_n t_1/\hbar} \delta_{nm}, \\ G_{0nm}^A(k; t_1 t_2) &= \frac{i}{\hbar} \theta(t_2 - t_1) e^{iE_m t_2/\hbar} e^{-iE_n t_1/\hbar} \delta_{nm}. \end{aligned} \quad (2.42)$$

2.5.2 Stationary Solution

Once the stationary solution of a nonequilibrium system is reached, the Green's functions $G_{nm}(\mathbf{k}_t; t t')$ do not depend on both t and t' , but only on the difference $t - t'$. Recalling that t and t' do not lie on an imaginary time contour (Langreth theorem) anymore, it is advantageous to make the Fourier transformation of the Green's functions with respect to the time difference $t - t'$. This will further simplify the equations

$$G_{nm}^<(\mathbf{k}_t; E) = \int dt (t - t') e^{iE(t-t')/\hbar} G_{nm}^<(\mathbf{k}_t; t - t') \quad (2.43)$$

and the inverse Fourier transformation

$$G_{nm}^<(\mathbf{k}_t; t - t') = \frac{1}{2\pi\hbar} \int dE e^{-iE(t-t')/\hbar} G_{nm}^<(\mathbf{k}_t; E). \quad (2.44)$$

The same relations hold for $G^{R,A}$. This produces simplified equations of motion for the stationary state of the system

$$\begin{aligned}
EG_{nm}^<(\mathbf{k}_t; E) - \sum_l h_{nl} G_{lm}^<(\mathbf{k}_t; E) &= \sum_l \Sigma_{nl}^R(\mathbf{k}_t; E) G_{lm}^<(\mathbf{k}_t; E) + \sum_l \Sigma_{nl}^<(\mathbf{k}_t; E) G_{lm}^A(\mathbf{k}_t; E) \\
EG_{nm}^<(\mathbf{k}_t; E) - \sum_l G_{nl}^<(\mathbf{k}_t; E) h_{lm} &= \sum_l G_{nl}^R(\mathbf{k}_t; E) \Sigma_{lm}^<(\mathbf{k}_t; E) + \sum_l G_{nl}^<(\mathbf{k}_t; E) \Sigma_{lm}^A(\mathbf{k}_t; E) \\
G_{nm}^<(\mathbf{k}_t; E) &= \sum_{l,v} G_{nl}^R(\mathbf{k}_t; E) \Sigma_{lv}^<(\mathbf{k}_t; E) G_{vm}^A(\mathbf{k}_t; E) \\
G_{nm}^<(\mathbf{k}_t; E) &= -[G_{mn}^<(\mathbf{k}_t; E)]^\dagger \\
EG_{nm}^R(\mathbf{k}_t; E) - \sum_l h_{nl} G_{lm}^R(\mathbf{k}_t; E) &= \delta_{nm} + \sum_l \Sigma_{nl}^R(\mathbf{k}_t; E) G_{lm}^R(\mathbf{k}_t; E) \\
G_{nm}^A(\mathbf{k}_t; E) &= [G_{mn}^R(\mathbf{k}_t; E)]^\dagger \\
G_{mn}^R(\mathbf{k}_t; E) - G_{mn}^A(\mathbf{k}_t; E) &= G_{mn}^>(\mathbf{k}_t; E) - G_{mn}^<(\mathbf{k}_t; E) \\
A(\mathbf{k}_t; E) &= i(G_{mn}^R(\mathbf{k}_t; E) - G_{mn}^A(\mathbf{k}_t; E))
\end{aligned}$$

(2.45)

Equation (2.45) forms a coupled system of equations, where $G^<$ and G^R have to be found. It also remains to determine the self-energies $\Sigma_{nm}^<(\mathbf{k}_t; E)$ and $\Sigma_{nm}^R(\mathbf{k}_t; E)$ for the different interactions present in the device. This can be found in [1, 15, 5, 4, 3] for example.

One considers a problem where there are N_L lattice points, N_k wavevector k points, N_E energy points, and the Hamiltonian h is a $N_H \times N_H$ matrix (tight-binding model). In this case, $N_L \times N_L \times N_k \times N_E \times N_H \times N_H$ functions G^R , $G^<$, Σ^R , and $\Sigma^<$ must be calculated and stored.

- An initial value for G^R and $G^<$ is required, for example the free Green's function G^{0R} and $G^{0<}$, when no interactions are present in the system.
- The self-energies Σ^R and $\Sigma^<$ are calculated with the actual G^R and $G^<$ for all the lattice, k , E , and H points.
- The values of the self-energies Σ^R and $\Sigma^<$ are then used to calculate a new G^R and $G^<$. This is done until convergence is achieved with Jacobi iterations for example.
- To take into account the carrier-carrier interactions on a mean-field level, the Poisson equation is solved with the actual carrier density obtained with $G^<$.

The algorithm starts again with the new calculated potential until it does not change anymore.

Thus, the calculation of current and carrier density with the help of Green's functions is very expensive and requires a lot of time. It can be accelerated by neglecting some parts of the self energies as shown in the application section and by parallelizing the computation of the self-energies.

2.5.3 Self-Energies Examples

The goal of this section is to describe different scattering mechanisms, first by giving their Hamiltonian and then the corresponding self-energy (obtained from the Wick's decomposition, the Feynman diagrams or the variational derivation). The different forms (lesser, greater, retarded, advanced) of the self-energies will be given as well as their eigenfunction expansion for transport in one direction (z) and plane-waves with the wavevector $\mathbf{k} = (k_x, k_y)$ in the other transverse directions.

2.5.3.1 Carrier-Carrier Interaction [2]

The Hamiltonian for carrier-carrier interaction is defined in equation (D.6)

$$H_{cc} = \frac{1}{2} \int dx_1 \int dx_2 \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) V(x_1 - x_2) \hat{\psi}(x_2) \hat{\psi}(x_1), \quad (2.46)$$

where $\hat{\psi}^\dagger$ and $\hat{\psi}$ are creation and annihilation operators, respectively. In Appendix F, it is shown that this Hamiltonian leads to an infinite number of self-energies, where one will retain the three first, the Hartree, Fock, and direct collision self-energies.

$$\begin{aligned} \Sigma^{Hartree}(12) &= -i\hbar\delta(12) \int d3 V(1-3)G(33^+) \\ \Sigma^{Fock}(12) &= i\hbar V(1-2)G(12) \\ \Sigma^{dc}(12) &= i\hbar \int d3 \int d4 V(2-3)\pi(34)W(41)G(12) \\ &= i\hbar \int d3 \int d4 V(2-3) (-i\hbar G(34)G(43^+)) W(41)G(12) \end{aligned} \quad (2.47)$$

with

$$\Sigma^{Fock}(12) + \Sigma^{dc}(12) = i\hbar W(21)G(12). \quad (2.48)$$

$\Sigma^{Hartree}(12)$ and $\Sigma^{Fock}(12)$ are instantaneous and build a singular part of the total self-energy. Furthermore, $\Sigma^{Hartree}(12)$ does not appear anymore explicitly in the Dyson's equations, it is included in the potential $U_{eff}(1)$, as shown in Appendix F, used to calculate the band bending

$$U_{eff}(1) = U(1) - i\hbar \int d2 V(1-2)G(22^+)$$

$$\begin{aligned}
&= U(1) + \int d^3 \mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) n(\mathbf{r}_2 t) \\
&= U(1) - \frac{1}{e} \int d^3 \mathbf{r}_2 \frac{e^2}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|} \rho(\mathbf{r}_2 t), \quad n(\mathbf{r}_2 t) = -\frac{1}{e} \rho(\mathbf{r}_2 t) \\
&= U(1) - e\phi(1),
\end{aligned} \tag{2.49}$$

where the potential $\phi(1)$ generates the following equations

$$\begin{aligned}
\phi(1) &= \int d^3 \mathbf{r}_2 \frac{1}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|} \rho(\mathbf{r}_2 t) \\
\mathbf{E}(1) &= -\text{grad } \phi(1) = \int d^3 \mathbf{r}_2 \frac{\mathbf{r}_1 - \mathbf{r}_2}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|^3} \rho(\mathbf{r}_2 t) \\
\int \mathbf{E}(1) \cdot d\mathbf{A} &= \int d^3 \mathbf{r}_1 \text{div } \mathbf{E}(1) = \int d^3 \mathbf{r}_2 \int \frac{d\mathbf{A} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|^3} \rho(\mathbf{r}_2 t) \\
&= \int d^3 \mathbf{r}_2 \int \frac{dA |\mathbf{r}_1 - \mathbf{r}_2|}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|^3} \rho(\mathbf{r}_2 t) \\
&= \int d^3 \mathbf{r}_2 \int_0^\pi d\theta \int_0^{2\pi} d\phi |\mathbf{r}_1 - \mathbf{r}_2|^2 \sin(\theta) \frac{1}{4\pi\epsilon |\mathbf{r}_1 - \mathbf{r}_2|^2} \rho(\mathbf{r}_2 t) \\
&= \int d^3 \mathbf{r}_2 \frac{\rho(\mathbf{r}_2 t)}{\epsilon} \\
\Rightarrow \text{div } \mathbf{E}(1) &= -\text{div grad } \phi(1) = \frac{\rho(1)}{\epsilon}.
\end{aligned}$$

The potential $\phi(1)$ resulting from the Hartree self-energy is in fact the solution of Poisson's equation induced by the charge density $\rho(1)$ present in the device.

Since $\Sigma^{\text{Hartree}}(12)$ is treated separately, one will consider only the eigenfunction expansion of $\Sigma^{FDC}(12) = \Sigma^{\text{Fock}}(12) + \Sigma^{dc}(12)$

$$\boxed{\Sigma_{nm}^{FDC}(\mathbf{k}; t_1 t_2) = i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} W_{nmn_1 m_1}(\mathbf{q}; t_2 t_1) G_{n_1 m_1}(\mathbf{k} + \mathbf{q}; t_1 t_2)} \tag{2.50}$$

where the inclusion of equation (F.13) delivers

$$\begin{aligned}
W_{nmn_1 m_1}(\mathbf{q}; t_2 t_1) &= V_{nmn_1 m_1}(\mathbf{q}; t_2 t_1) + \sum_{n_3 m_3 n_4 m_4} \sum_{\mathbf{k}_1} \int dt_3 \int dt_4 V_{m_4 m n_3 m_1}(\mathbf{q}; t_2 t_3) \\
&\quad \times \pi_{n_3 m_3 n_4 m_4}(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{q}; t_3 t_4) W_{nn_4 n_1 m_3}(\mathbf{q}; t_4 t_1),
\end{aligned} \tag{2.51}$$

$$V_{nmn_1 m_1}(\mathbf{q}; t_2 t_1) = \frac{1}{A} \int d(\mathbf{r}_{\mathbf{xy}1} - \mathbf{r}_{\mathbf{xy}2}) \int dz_1 \int dz_2 \phi_n^*(z_1) \phi_m(z_2) V(2-1) \phi_{n_1}(z_1) \phi_{m_1}^*(z_2) e^{-i\mathbf{q}(\mathbf{r}_{\mathbf{xy}2} - \mathbf{r}_{\mathbf{xy}1})},$$

$$W_{nmn_1 m_1}(\mathbf{q}; t_2 t_1) = \frac{1}{A} \int d(\mathbf{r}_{\mathbf{xy}1} - \mathbf{r}_{\mathbf{xy}2}) \int dz_1 \int dz_2 \phi_n^*(z_1) \phi_m(z_2) W(21) \phi_{n_1}(z_1) \phi_{m_1}^*(z_2) e^{-i\mathbf{q}(\mathbf{r}_{\mathbf{xy}2} - \mathbf{r}_{\mathbf{xy}1})},$$

$$\pi_{n_3 m_3 n_4 m_4}(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{q}; t_3 t_4) = -i\hbar G_{n_3 m_3}(\mathbf{k}_1; t_3 t_4) G_{n_4 m_4}(\mathbf{k}_1 - \mathbf{q}; t_4 t_3), \quad (2.52)$$

$\mathbf{q} = (q_x, q_y)$, and $\mathbf{k}_1 = (k_{1x}, k_{1y})$. For the Fock self-energy only, one has

$$\boxed{\begin{aligned} \Sigma_{nm}^{Fock}(\mathbf{k}; t_1 t_2) &= \delta(t_1 - t_2) i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} V_{nm n_1 m_1}(\mathbf{q}) G_{n_1 m_1}(\mathbf{k} + \mathbf{q}; t_1 t_1^+) \\ &= \delta(t_1 - t_2) i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} V_{nm n_1 m_1}(\mathbf{q}) G_{n_1 m_1}^<(\mathbf{k} + \mathbf{q}; t_1 t_1). \end{aligned}}$$

The lesser and greater self-energies are obtained from equation (2.50), where the Fock part is not considered because it is instantaneous

$$\boxed{\Sigma_{nm}^{dc<}(\mathbf{k}; t_1 t_2) = i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} W_{nm n_1 m_1}^>(\mathbf{q}; t_2 t_1) G_{n_1 m_1}^<(\mathbf{k} + \mathbf{q}; t_1 t_2).} \quad (2.53)$$

$\Sigma_{nm}^{dc>}(\mathbf{k}; t_1 t_2)$ is calculated by inverting $<$ and $>$. It remains to determine $W_{nm n_1 m_1}^>$. From equation (2.51), one finds by neglecting the indices

$$W^>(t_2 t_1) = \int dt_3 \int dt_4 V(t_2 t_3) \pi^R(t_3 t_4) W^>(t_4 t_1) + \int dt_3 \int dt_4 V(t_2 t_3) \pi^>(t_3 t_4) W^A(t_4 t_1).$$

This implies that

$$\int dt_4 \underbrace{(\delta(24) - \int dt_3 V(t_2 t_3) \pi^R(t_3 t_4))}_{\epsilon^R(t_2 t_4) = \left(\frac{dU_{eff}(t_2)}{dU(t_4)} \right)^{-1}} W^>(t_4 t_1) = \int dt_3 \int dt_4 V(t_2 t_3) \pi^>(t_3 t_4) W^A(t_4 t_1),$$

which can be proved by using equations (F.12), (F.42), and (F.44). These considerations enable to write

$$\underbrace{\int dt_2 \int dt_4 [\epsilon^R(t' t_2)]^{-1} \epsilon^R(t_2 t_4) W^>(t_4 t_1)}_{W^>(t' t_1)} = \int dt_3 \int dt_4 \underbrace{\int dt_2 [\epsilon^R(t' t_2)]^{-1} V(t_2 t_3) \pi^>(t_3 t_4) W^A(t_4 t_1)}_{W^R(t' t_3)}$$

and the final result

$$W_{nm n_1 m_1}^>(\mathbf{q}; t_2 t_1) = \sum_{n_3 m_3 n_4 m_4} \sum_{\mathbf{k}_1} \int dt_3 \int dt_4 W_{m_4 m n_3 m_1}^R(\mathbf{q}; t_2 t_3) \pi_{n_3 m_3 n_4 m_4}^>(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{q}; t_3 t_4) W_{nn_4 n_1 m_3}^A(\mathbf{q}; t_4 t_1).$$

The procedure to get $W^{R,A}$ and $\pi^>$ is similar to the one needed for $W^>$ and can be found in [2, 13]. For the stationary case, all the variables depend only on their time difference and a Fourier transformation of it as described in section 2.5.2 is very useful. This yields for the direct collision self-energy

$$\boxed{\Sigma_{nm}^{dc<}(\mathbf{k}; E) = i \int \frac{dE'}{2\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} W_{nm n_1 m_1}^>(\mathbf{q}; E') G_{n_1 m_1}^<(\mathbf{k} + \mathbf{q}; E - E').} \quad (2.54)$$

The energy-dependent screened interaction $W^>(E')$ is given by

$$W_{nm n_1 m_1}^>(\mathbf{q}; E') = \sum_{n_3 m_3 n_4 m_4} \sum_{\mathbf{k}_1} W_{m_4 m n_3 m_1}^R(\mathbf{q}; E') \pi_{n_3 m_3 n_4 m_4}^>(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{q}; E') W_{nn_4 n_1 m_3}^A(\mathbf{q}; E')$$

with

$$\pi_{n_3 m_3 n_4 m_4}^>(\mathbf{k}_1, \mathbf{k}_1 - \mathbf{q}; E') = -i \int \frac{dE''}{2\pi} G_{n_3 m_3}^>(\mathbf{k}_1; E'') G_{n_4 m_4}^<(\mathbf{k}_1 - \mathbf{q}; E'' - E').$$

The retarded or advanced component of the self-energy can be obtained from the definition

$$\Sigma^{R,A}(12) = \Sigma^\delta(12) \pm \theta(\pm t \mp t') [\Sigma^>(12) - \Sigma^<(12)] \quad (2.55)$$

which can also be expanded into eigenfunctions or Fourier transformed.

2.5.3.2 Carrier-Optical-Phonon Interaction [3]

The Hamiltonian describing carrier-optical-phonon interaction has the following form (see equation (F.57))

$$H^{FR} = \int dr \hat{\psi}^\dagger(r) \sum_q \frac{e^{iqr}}{|q|} (C a_q + C^* a_{-q}^\dagger) \hat{\psi}(r), \quad (2.56)$$

where a_q and a_{-q}^\dagger are the phonon annihilation and creation operators, respectively, and

$$C = i \sqrt{\frac{e^2 \hbar \omega_{LO}}{V} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)}. \quad (2.57)$$

C is the Fröhlich coupling constant. Using Wick's decomposition or the second Feynman diagrams in equation (E.22), one obtains for the self-energy (Appendix F, eq. (F.68))

$$\Sigma^{ph}(12) = i\hbar |C|^2 \sum_{\mathbf{q}_1 \mathbf{q}_2} \frac{e^{i\mathbf{q}_1 \mathbf{r}_1} e^{i\mathbf{q}_2 \mathbf{r}_2}}{|\mathbf{q}_1| |\mathbf{q}_2|} D(\mathbf{q}_1 \mathbf{q}_2; t_1 t_2) G(12), \quad (2.58)$$

with, derived from equation (F.62),

$$D(\mathbf{q}_1 \mathbf{q}_1; t_1 t_2) = -\frac{i}{\hbar} \frac{\langle T \{ S [a_{\mathbf{q}_1}(t_1) a_{-\mathbf{q}_2}^\dagger(t_2) + a_{-\mathbf{q}_1}^\dagger(t_1) a_{\mathbf{q}_2}(t_2)] \} \rangle}{\langle S \rangle} \delta_{\mathbf{q}_1, -\mathbf{q}_2}. \quad (2.59)$$

The eigenfunction expansion of (2.58) yields

$$\Sigma_{nm}^{ph}(\mathbf{k}; t_1 t_2) = i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) D(\mathbf{q}; t_1 t_2) G_{n_1 m_1}(\mathbf{k} - \mathbf{q}; t_1 t_2) \quad (2.60)$$

where the form factor $M_{nn_1}(\mathbf{q})$ and $D(\mathbf{q}; t_1 t_2)$ are

$$M_{nn_1}(\mathbf{q}) = \left| \frac{C}{\mathbf{q}} \right| \int dz \phi_n^*(z) e^{iqz} \phi_{n_1}(z) \quad \text{and} \quad D(\mathbf{q}; t_1 t_2) = D(\mathbf{q}, -\mathbf{q}; t_1 t_2).$$

To find the lesser and the retarded self-energies, Langreth theorem from section 2.3 is applied

$$\begin{aligned}
\Sigma_{nm}^{<ph}(\mathbf{k}; t_1 t_2) &= i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) D^<(\mathbf{q}; t_1 t_2) G_{n_1 m_1}^<(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2) \\
\Sigma_{nm}^{Rph}(\mathbf{k}; t_1 t_2) &= i\hbar \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) \{ D^R(\mathbf{q}; t_1 t_2) G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2) \\
&\quad + D^R(\mathbf{q}; t_1 t_2) G_{n_1 m_1}^<(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2) + D^<(\mathbf{q}; t_1 t_2) G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2) \}
\end{aligned} \tag{2.61}$$

and after a Fourier transformation for steady-state, one gets

$$\begin{aligned}
\Sigma_{nm}^{<ph}(\mathbf{k}; E) &= i \sum_{n_1 m_1} \sum_{\mathbf{q}} \int \frac{dE'}{2\pi} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) D^<(\mathbf{q}; E') G_{n_1 m_1}^<(\mathbf{k} - \mathbf{q}_{||}; E - E') \\
\Sigma_{nm}^{Rph}(\mathbf{k}; E) &= i \sum_{n_1 m_1} \sum_{\mathbf{q}} \int \frac{dE'}{2\pi} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) \{ D^R(\mathbf{q}; E') G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; E - E') \\
&\quad + D^R(\mathbf{q}; E') G_{n_1 m_1}^<(\mathbf{k} - \mathbf{q}_{||}; E - E') + D^<(\mathbf{q}; E') G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; E - E') \}.
\end{aligned} \tag{2.62}$$

For a complete set of equations Dyson's equation for the phonon Green's function $D(\mathbf{q}; E)$ should be solved, but it is more convenient to assume that the phonon bath is in equilibrium so that the free phonon Green's functions $D^{(0)}(\mathbf{q}; E)$ from equation (F.64) can replace $D(\mathbf{q}; E)$. Thus one will use the following expressions

$$\begin{aligned}
D^R(\mathbf{q}; E') &= \frac{1}{E' - \hbar\omega_{\mathbf{q}} + i\delta} - \frac{1}{E' + \hbar\omega_{\mathbf{q}} + i\delta} \\
D^<(\mathbf{q}; E') &= -2\pi i [N_{\mathbf{q}}\delta(E' - \hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}} + 1)\delta(E' + \hbar\omega_{\mathbf{q}})].
\end{aligned} \tag{2.63}$$

$N_{\mathbf{q}}$ is the Bose distribution for the phonons and $\omega_{\mathbf{q}}$ the phonon frequency. One has four different integrals to evaluate to obtain both self-energies. For the retarded component of the phonon Green's function D^R , one applies the property

$$\frac{1}{x + i\delta} = -i\pi\delta(x) + \mathcal{P} \left\{ \frac{1}{x} \right\}. \tag{2.64}$$

The results are

$$\begin{aligned}
i \int \frac{dE'}{2\pi} D^<(\mathbf{q}; E') G^<(\mathbf{k} - \mathbf{q}_{||}; E - E') &= \int dE' G^<(\mathbf{k} - \mathbf{q}_{||}; E - E') [N_{\mathbf{q}}\delta(E' - \hbar\omega_{\mathbf{q}}) \\
&\quad + (N_{\mathbf{q}} + 1)\delta(E' + \hbar\omega_{\mathbf{q}})] \\
&= N_{\mathbf{q}} G^<(\mathbf{k} - \mathbf{q}_{||}; E - \hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}} + 1) G^<(\mathbf{k} - \mathbf{q}_{||}; E + \hbar\omega_{\mathbf{q}}) \\
i \int \frac{dE'}{2\pi} D^<(\mathbf{q}; E') G^R(\mathbf{k} - \mathbf{q}_{||}; E - E') &= N_{\mathbf{q}} G^R(\mathbf{k} - \mathbf{q}_{||}; E - \hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}} + 1) G^R(\mathbf{k} - \mathbf{q}_{||}; E + \hbar\omega_{\mathbf{q}}) \\
i \int \frac{dE'}{2\pi} D^R(\mathbf{q}; E') G^<(\mathbf{k} - \mathbf{q}_{||}; E - E') &= \frac{1}{2} \int dE' G^<(\mathbf{k} - \mathbf{q}_{||}; E - E') [\delta(E' - \hbar\omega_{\mathbf{q}}) - \delta(E' + \hbar\omega_{\mathbf{q}})]
\end{aligned}$$

$$\begin{aligned}
& + i\mathcal{P} \left\{ \int \frac{dE'}{2\pi} \left(\frac{G^<(E-E')}{E'-\hbar\omega_{\mathbf{q}}} - \frac{G^<(E-E')}{E'+\hbar\omega_{\mathbf{q}}} \right) \right\} \\
i \int \frac{dE'}{2\pi} D^R(E') G^R(E-E') &= i \int \frac{dE'}{2\pi} \left(\frac{G^R(E-E')}{E'-\hbar\omega_{\mathbf{q}}+i\delta} - \frac{G^R(E-E')}{E'+\hbar\omega_{\mathbf{q}}+i\delta} \right) \\
&= G^R(E-\hbar\omega_{\mathbf{q}}) - G^R(E+\hbar\omega_{\mathbf{q}}).
\end{aligned}$$

The last integral solution is obtained because $G^R(E-E')$ has only poles for $\Im(E-E') < 0$ or $\Im(E') > 0$, due to the $\theta(t-t')$ factor present in equation (1.26). Hence, it is possible to integrate with a loop containing the lower part of the complex plane, where the only pole is $\hbar\omega_{\mathbf{q}} - i\delta$ for the first part of the integral and $-\hbar\omega_{\mathbf{q}} - i\delta$ for the second. This is done with the residue theorem without forgetting that a contour integral in the lower part of the complex plane yields a negative sign and a contour integral in the positive plane a positive sign. Finally, the self-energies become

$$\begin{aligned}
\Sigma_{nm}^{<ph}(\mathbf{k}; E) &= \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) \{ N_{\mathbf{q}} G^<(\mathbf{k}-\mathbf{q}_{||}; E-\hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}}+1) G^<(\mathbf{k}-\mathbf{q}_{||}; E+\hbar\omega_{\mathbf{q}}) \} \\
\Sigma_{nm}^{Rph}(\mathbf{k}; E) &= \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) [(N_{\mathbf{q}}+1) G^R(\mathbf{k}-\mathbf{q}_{||}; E-\hbar\omega_{\mathbf{q}}) + N_{\mathbf{q}} G^R(\mathbf{k}-\mathbf{q}_{||}; E+\hbar\omega_{\mathbf{q}}) \\
&\quad + \frac{1}{2} (G^<(\mathbf{k}-\mathbf{q}_{||}; E-\hbar\omega_{\mathbf{q}}) - G^<(\mathbf{k}-\mathbf{q}_{||}; E+\hbar\omega_{\mathbf{q}})) \\
&\quad + i\mathcal{P} \left\{ \int \frac{dE'}{2\pi} \left(\frac{G^<(\mathbf{k}-\mathbf{q}_{||}; E-E')}{E'-\hbar\omega_{\mathbf{q}}} - \frac{G^<(\mathbf{k}-\mathbf{q}_{||}; E-E')}{E'+\hbar\omega_{\mathbf{q}}} \right) \right\}] \\
\Sigma_{nm}^{Aph}(\mathbf{k}; E) &= \sum_{n_1 m_1} \sum_{\mathbf{q}} M_{nn_1}(\mathbf{q}) M_{mm_1}^*(\mathbf{q}) [(N_{\mathbf{q}}+1) G^A(\mathbf{k}-\mathbf{q}_{||}; E-\hbar\omega_{\mathbf{q}}) + N_{\mathbf{q}} G^A(\mathbf{k}-\mathbf{q}_{||}; E+\hbar\omega_{\mathbf{q}}) \\
&\quad + \frac{1}{2} (G^<(\mathbf{k}-\mathbf{q}_{||}; E+\hbar\omega_{\mathbf{q}}) - G^<(\mathbf{k}-\mathbf{q}_{||}; E-\hbar\omega_{\mathbf{q}})) \\
&\quad + i\mathcal{P} \left\{ \int \frac{dE'}{2\pi} \left(\frac{G^<(\mathbf{k}-\mathbf{q}_{||}; E-E')}{E'-\hbar\omega_{\mathbf{q}}} - \frac{G^<(\mathbf{k}-\mathbf{q}_{||}; E-E')}{E'+\hbar\omega_{\mathbf{q}}} \right) \right\}].
\end{aligned} \tag{2.65}$$

The details for the advanced self-energy $\Sigma_{nm}^{Aph}(\mathbf{k}; E)$ are not given, but the procedure is the same as for $\Sigma_{nm}^{Rph}(\mathbf{k}; E)$, starting with equation (2.22).

2.5.3.3 Carrier-Acoustic-Phonon Interaction [4]

The Hamiltonian for carrier-acoustic-phonon interaction looks like the one for carrier-optical-phonon

$$H^{acph} = \int dr \hat{\psi}^\dagger(r) \sum_{\mathbf{q}} e^{i\mathbf{q}r} |\mathbf{q}| \left(U a_{\mathbf{q}} + U^* a_{-\mathbf{q}}^\dagger \right) \hat{\psi}(r) \tag{2.66}$$

where $a_{\mathbf{q}}$ and $a_{-\mathbf{q}}^\dagger$ are the annihilation and creation phonon operators, respectively, and $U = i\sqrt{\frac{\hbar D^2}{2V\rho c_s}}$. D is the material deformation potential, ρ the semiconductor

density, V the volume, and c_s the velocity of sound in the crystal. As consequence, one obtains the same self-energies as for the carrier-optical-phonon interaction except for the form factor $M_{nn_1}(\mathbf{q})$

$$M_{nn_1}(\mathbf{q}) = |U||\mathbf{q}| \int dz \phi_n^*(z) e^{iq_z z} \phi_{n_1}(z) = |U||\mathbf{q}| M'_{nn_1}(q_z) \quad (2.67)$$

which is slightly different. In contradiction to the previous section, it is possible to simplify the resulting carrier-acoustic-phonon self-energies by assuming that the phonon frequency $\omega_{\mathbf{q}}$ is small. One has therefore

$$\omega_{\mathbf{q}} = c_s |\mathbf{q}|, \quad N_{\mathbf{q}} = \frac{1}{e^{\hbar\omega_{\mathbf{q}}/(k_B T)} - 1} \approx \frac{k_B T}{\hbar\omega_{\mathbf{q}}} \approx N_{\mathbf{q}} + 1, \quad E' \pm \hbar\omega_{\mathbf{q}} = E'. \quad (2.68)$$

These assumptions lead to the following expressions

$$\begin{aligned} \Sigma_{nm}^{<ac}(\mathbf{k}; E) &= \frac{D^2 k_B T}{V \rho c_s^2} \sum_{n_1 m_1} \sum_{\mathbf{q}} M'_{nn_1}(q_z) M_{mm_1}^*(q_z) G_{n_1 m_1}^{<}(\mathbf{k} - \mathbf{q}_{||}; E) \\ \Sigma_{nm}^{Rac}(\mathbf{k}; E) &= \frac{D^2 k_B T}{V \rho c_s^2} \sum_{n_1 m_1} \sum_{\mathbf{q}} M'_{nn_1}(q_z) M_{mm_1}^*(q_z) G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; E). \end{aligned} \quad (2.69)$$

With the above simplifications, the self-energies for carrier-acoustic-phonon interaction are elastic because there is no energy exchange during the phonon absorption or emission process.

2.5.3.4 Impurity Scattering [5]

Impurity scattering is an interaction between a moving carrier and a fix ionized atom. Its Hamiltonian is given by

$$H^{is} = \sum_i \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) V(\mathbf{r} - \mathbf{R}_i) \hat{\psi}(\mathbf{r}), \quad (2.70)$$

where $\hat{\psi}^\dagger$ and $\hat{\psi}$ are creation and annihilation operators, respectively, and $V(\mathbf{r} - \mathbf{R}_i)$ is the potential describing the interaction between a carrier at site \mathbf{r} and an impurity at site \mathbf{R}_i . The potential can be expressed through its inverse Fourier transform

$$V(\mathbf{r} - \mathbf{R}_i) = \frac{1}{V} \sum_{\mathbf{q}} V(\mathbf{q}) e^{i\mathbf{q}(\mathbf{r} - \mathbf{R}_i)}, \quad (2.71)$$

where $V(\mathbf{q})$ is the Fourier transformation of $V(\mathbf{r})$ and V the volume. The Wick's decomposition described in Appendix D gives the following expression for the impurity scattering self-energy, if one retains only the second order perturbation

$$\Sigma^{is}(12) = \frac{1}{V^2} \sum_{\mathbf{q}_1 \mathbf{q}_2} V(\mathbf{q}_1) V(\mathbf{q}_2) e^{i\mathbf{q}_1 \mathbf{r}_1} e^{i\mathbf{q}_2 \mathbf{r}_2} \left\langle \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \right\rangle G(12) \quad (2.72)$$

The brackets $\langle \rangle$ mean that the quantity in the middle must be statistically averaged

$$\langle \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \rangle = \langle \sum_{i=j} e^{-i(\mathbf{q}_1 + \mathbf{q}_2) \mathbf{R}_i} \rangle + \langle \sum_{i \neq j} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \rangle \quad (2.73)$$

Obviously, the first term is only different from zero if $\mathbf{q}_1 + \mathbf{q}_2 = 0$, the second if $\mathbf{q}_1 = \mathbf{q}_2 = 0$. The result is then

$$\langle \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \rangle = N_i \delta_{\mathbf{q}_1 + \mathbf{q}_2 = 0} + \underbrace{N_i(N_i - 1) \delta_{\mathbf{q}_1 = 0} \delta_{\mathbf{q}_2 = 0}}_{\text{neglected}} \quad (2.74)$$

where N_i is the number of impurities present in the device. The second term is neglected because it has less importance than the first one. The self-energy is then

$$\boxed{\begin{aligned} \Sigma^{is}(12) &= \frac{N_i}{V^2} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} G(12) \\ &= \frac{\rho}{V} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} G(12). \end{aligned}} \quad (2.75)$$

ρ is the impurity density. The eigenfunction expansion of equation (2.75) and the consideration of the lesser and retarded part of the self-energies yields

$$\boxed{\begin{aligned} \Sigma_{nm}^{is}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{V} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{nn_1}(q_z) M'^*_{mm_1} G_{n_1 m_1}(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2). \\ \Sigma_{nm}^{<is}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{V} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{nn_1}(q_z) M'^*_{mm_1} G_{n_1 m_1}^{<}(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2). \\ \Sigma_{nm}^{Ris}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{V} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{nn_1}(q_z) M'^*_{mm_1} G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; t_1 t_2). \end{aligned}} \quad (2.76)$$

The matrix elements $M'_{nn_1}(q_z)$ and $M'^*_{mm_1}$ are defined in equation (2.67). For stationary regime, where the Green's functions and the self-energies depend only on time differences, a Fourier transform leads to

$$\boxed{\begin{aligned} \Sigma_{nm}^{<is}(\mathbf{k}; E) &= \frac{\rho}{V} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{nn_1}(q_z) M'^*_{mm_1} G_{n_1 m_1}^{<}(\mathbf{k} - \mathbf{q}_{||}; E). \\ \Sigma_{nm}^{Ris}(\mathbf{k}; E) &= \frac{\rho}{V} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{nn_1}(q_z) M'^*_{mm_1} G_{n_1 m_1}^R(\mathbf{k} - \mathbf{q}_{||}; E). \end{aligned}} \quad (2.77)$$

The other scattering mechanisms mentioned in this report like alloy disorder, or interface roughness are very similar to impurity scattering in the way they are calculated: each time, there is a potential $V(\mathbf{r}, \mathbf{R})$ depending on the carrier position \mathbf{r} and on another quantity (dopant or roughness amplitude...) at position \mathbf{R} which must be statistically averaged.

2.6 Boundary Conditions [3]

In order to solve the above defined system, boundary conditions have to be specified. An important point is the treatment of equilibrated contacts, which act as a source or drain for the electric current. For that purpose, one considers equation (2.45), first of all for the retarded Green's function G^R . As it is obvious, this equation can be written as a matrix equation, where one separates the system into submatrices: a central region with index C and a lead region with index L . Then the matrix equation (2.45) can be written in the form

$$\begin{pmatrix} E - h_{CC} + i0^+ & 0 \\ 0 & E - h_{LL} + i0^+ \end{pmatrix} \cdot \begin{pmatrix} G_{CC}^R & G_{CL}^R \\ G_{LC}^R & G_{LL}^R \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \left[\begin{pmatrix} U_{CC} & U_{CL} \\ U_{LC} & U_{LL} \end{pmatrix} + \begin{pmatrix} \Sigma_{CC}^R & 0 \\ 0 & \Sigma_{LL}^R \end{pmatrix} \right] \cdot \begin{pmatrix} G_{CC}^R & G_{CL}^R \\ G_{LC}^R & G_{LL}^R \end{pmatrix} \quad (2.78)$$

where all the functions are matrices, Σ_{CL} and Σ_{LC} are neglected, h_{CC} and h_{LL} are diagonal matrices corresponding to h_{nm} in equation (2.45) and the U 's are the other elements $h_{nm}, n \neq m$, $E - h_{CC} + i0^+ = \tilde{G}_{0C}^{-1}$, and $E - h_{LL} + i0^+ = \tilde{G}_{0L}^{-1}$. \tilde{G}_{0C} and \tilde{G}_{0L} are not the non-interacting Green's functions in the device and in the lead, respectively but just help variables. Starting with the equation for G_{LC}^R , one obtains

$$\tilde{G}_{0L}^{-1} G_{LC}^R = U_{LC} G_{CC}^R + (U_{LL} + \Sigma_{LL}^R) G_{LC}^R \quad (2.79)$$

or

$$\begin{aligned} G_{LC}^R &= \tilde{G}_{0L} U_{LC} G_{CC}^R + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) G_{LC}^R \\ &= (\tilde{G}_{0L} + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} \\ &\quad + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} + \dots) U_{LC} G_{CC}^R \\ &= g_{LL}^R U_{LC} G_{CC}^R, \end{aligned} \quad (2.80)$$

where the second line is obtained by reiterating G_{LC}^R . g_{LL}^R is the lead Green's function when the lead and the device are separated (but to compute Σ_{LL} , the Green's functions in the device should be known)

$$g_{LL}^R = \tilde{G}_{0L} + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) g_{LL}^R. \quad (2.81)$$

The equation for G_{CC}^R is given by

$$\begin{aligned} G_{CC}^R &= \tilde{G}_{0C} + \tilde{G}_{0C} U_{CC} G_{CC}^R + \tilde{G}_{0C} U_{CL} G_{LC}^R + \tilde{G}_{0C} \Sigma_{CC} G_{CC}^R \\ &= \tilde{G}_{0C} (1 + U_{CL} G_{LC}^R) + \tilde{G}_{0C} (U_{CC} + \Sigma_{CC}) G_{CC}^R \\ &= g_{CC}^R (1 + U_{CL} G_{LC}^R) \\ &= g_{CC}^R + g_{CC}^R U_{CL} g_{LL}^R U_{LC} G_{CC}^R. \end{aligned} \quad (2.82)$$

The third equality results from the same procedure as for G_{LC}^R where g_{CC}^R is the device Green's function when the leads are not coupled

$$g_{CC}^R = \tilde{G}_{0C} + \tilde{G}_{0C} (U_{CC} + \Sigma_{CC}^R) g_{CC}^R. \quad (2.83)$$

The iteration procedure gives the following expression for G_{LL}^R

$$G_{LL}^R = g_{LL}^R(1 + U_{LC}G_{CL}^R). \quad (2.84)$$

It remains to evaluate G_{CL}^R , for which one has to consider the commutative rule $HG^R = G^RH = I$

$$\begin{pmatrix} G_{CC}^R & G_{CL}^R \\ G_{LC}^R & G_{LL}^R \end{pmatrix} \cdot \begin{pmatrix} E - h_{CC} + i0^+ & 0 \\ 0 & E - h_{LL} + i0^+ \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ + \begin{pmatrix} G_{CC}^R & G_{CL}^R \\ G_{LC}^R & G_{LL}^R \end{pmatrix} \cdot \left[\begin{pmatrix} U_{CC} & U_{CL} \\ U_{LC} & U_{LL} \end{pmatrix} + \begin{pmatrix} \Sigma_{CC}^R & 0 \\ 0 & \Sigma_{LL}^R \end{pmatrix} \right]. \quad (2.85)$$

This gives for G_{CL}^R

$$\begin{aligned} G_{CL}^R &= G_{CC}^R U_{CL} \tilde{G}_{0L} + G_{CL}^R (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} \\ &= G_{CC}^R U_{CL} (\tilde{G}_{0L} + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} \\ &\quad + \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{G}_{0L} + \dots) \\ &= G_{CC}^R U_{CL} g_{LL}^R \end{aligned} \quad (2.86)$$

The contact properties are included in the lead Green's function g_{LL}^R , where one can assume equilibrium and thus that electrons and holes are governed by a Fermi distribution. This approach enables the definition of the boundary conditions for $G^<$, too [3]. This gives,

$$\begin{aligned} G_{CC}^< &= G_{CC}^R \Sigma_{CC}^< G_{CC}^A + G_{CL}^R \Sigma_{LL}^< G_{LC}^A \\ &= G_{CC}^R \Sigma_{CC}^< G_{CC}^A + G_{CC}^R U_{CL} \underbrace{g_{LL}^R \Sigma_{LL}^< g_{LL}^A}_{g_{LL}^<} U_{LC} G_{CC}^A \\ &= G_{CC}^R \Sigma_{CC}^< G_{CC}^A + G_{CC}^R U_{CL} g_{LL}^< U_{LC} G_{CC}^A \\ \\ G_{CL}^< &= G_{CC}^R \Sigma_{CC}^< G_{CL}^A + G_{CL}^R \Sigma_{LL}^< G_{LL}^A \\ &= \underbrace{G_{CC}^R \Sigma_{CC}^< G_{CC}^A}_{G_{CC}^<} U_{CL} g_{LL}^A + G_{CC}^R U_{CL} \underbrace{g_{LL}^R \Sigma_{LL}^< g_{LL}^A}_{g_{LL}^<} (1 + \underbrace{U_{LC} G_{CL}^A}_{\text{neglected}}) \\ &= G_{CC}^< U_{CL} g_{LL}^A + G_{CC}^R U_{CL} g_{LL}^< \\ \\ G_{LC}^< &= G_{LL}^R \Sigma_{LL}^< G_{LC}^A + G_{LC}^R \Sigma_{CC}^< G_{CC}^A \\ &= (1 + \underbrace{U_{LC} G_{CL}^R}_{\text{neglected}}) \underbrace{g_{LL}^R \Sigma_{LL}^< g_{LL}^A}_{g_{LL}^<} U_{LC} G_{CC}^A + g_{LL}^R U_{LC} \underbrace{G_{CC}^R \Sigma_{CC}^< G_{CC}^A}_{G_{CC}^<} \\ &= g_{LL}^< U_{LC} G_{CC}^A + g_{LL}^R U_{LC} G_{CC}^< \\ G_{LL}^< &= \underbrace{G_{LL}^R \Sigma_{LL}^< G_{LL}^A}_1 + \underbrace{G_{LC}^R \Sigma_{CC}^< G_{CL}^A}_2 \\ &= \underbrace{g_{LL}^R \Sigma_{LL}^< g_{LL}^A}_{1a} + \underbrace{g_{LL}^R U_{LC} G_{CC}^R U_{CL} g_{LL}^R \Sigma_{LL}^< g_{LL}^A}_{1b} + \end{aligned}$$

$$\begin{aligned}
& \underbrace{g_{LL}^R \Sigma_{LL}^< g_{LL}^A U_{LC} G_{CC}^A U_{CL} g_{LL}^A}_{1c} + \underbrace{g_{LL}^R U_{LC} G_{CC}^R \Sigma_{CC}^< G_{CC}^A U_{CL} g_{LL}^A}_{2} + \\
& \underbrace{g_{LL}^R U_{LC} G_{CC}^R U_{CL} g_{LL}^R \Sigma_{LL}^< g_{LL}^A U_{LC} G_{CC}^A U_{CL} g_{LL}^A}_{1d} \\
& = \underbrace{g_{LL}^<}_{1a} + \underbrace{2i\Im\{g_{LL}^R U_{LC} G_{CC}^R U_{CL} g_{LL}^<\}}_{1b+1c} + \underbrace{g_{LL}^R U_{LC} G_{CC}^< U_{CL} g_{LL}^A}_{1d+2} \quad (2.87)
\end{aligned}$$

A complete treatment of the boundary conditions is also given in [4, 14].

2.7 Current and Carrier Density[6, 7, 8]

The carrier density $n(r, t)$ as function of the Green's functions was already given in equation (1.32). This relation remains the same in nonequilibrium

$$n(r, t) = -i\hbar G^<(r, t; r, t). \quad (2.88)$$

Assuming a one-dimensional eigenfunction expansion (z) of the Green's functions and stationary regime, one finds for the carrier density with equations (2.25) and (2.44)

$$n(z) = -\frac{i}{A} \sum_{\mathbf{k}_t, \sigma} \sum_{nm} \int \frac{dE}{2\pi} G_{nm}^<(\mathbf{k}_t; E) \phi_{\mathbf{k}_t n}(z) \phi_{\mathbf{k}_t m}^*(z), \quad (2.89)$$

where σ represents both spin polarization. It is more complicated to determine the current than the carrier density. The starting point is the continuity equation relating the current density $J(z, t)$ to the carrier density $\rho(z, t)$

$$\frac{d}{dt} \rho(z, t) + \text{div } J(z, t) = 0. \quad (2.90)$$

The density $\rho(z, t)$ is directly related to the lesser Green's functions $G^< (11')$ with

$$\frac{d}{dt} \rho(z, t) = \lim_{t' \rightarrow t} (-i\hbar) e \left(\frac{d}{dt} G^<(z, t, z, t') + \frac{d}{dt'} G^<(z, t, z, t') \right). \quad (2.91)$$

Choosing eigenfunctions centered around one lattice point as described in [4] and assuming a current flowing in the z -direction enables to write equation (2.90) as

$$\begin{aligned}
\frac{d}{dt} \rho_n(t) &= \frac{e}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \frac{d}{dt} \langle a_{n, \mathbf{k}_t}^\dagger(t) a_{n, \mathbf{k}_t}(t) \rangle, \quad e>0 \text{ for h, } e<0 \text{ for el.} \\
&= \lim_{t' \rightarrow t} (-i\hbar) \frac{e}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \left(\frac{d}{dt} G_{nn}^<(\mathbf{k}_t; tt') + \frac{d}{dt'} G_{nn}^<(\mathbf{k}_t; tt') \right) \\
&= -\frac{J_n(t) - J_{n-1}(t)}{\Delta}, \quad (2.92)
\end{aligned}$$

where $a_{n, \mathbf{k}_t}^\dagger$ creates an electron at position z_n , state \mathbf{k}_t , and time t (within a volume $V = A\Delta$), $a_{n, \mathbf{k}_t}(t)$ annihilates an electron with the same properties, $\rho_n(t)$ and $J_n(t)$

are the charge and current density at place z_n , respectively, A the area in the xy plane, $\Delta = z_n - z_{n-1}$, and e is the charge, positive for holes, negative for electrons. In fact, $J_n(t)$ represents the current density for a point situated between n and $n + 1$.

To find an expression for the current density $J_n(t)$, the two derivatives of the lesser Green's function $G_{mn}^<(\mathbf{k}_t; tt')$ are required. They can be found in equations (2.34) and (2.35) and inserted into (2.92)

$$\begin{aligned}
\frac{d}{dt}\rho_n(t) &= -\frac{e}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \sum_m \{ (h_{nm} G_{mn}^<(\mathbf{k}_t; tt) - G_{nm}^<(\mathbf{k}_t; tt) h_{mn}) + \\
&\quad \int dt_2 \left([\Sigma_{nm}^R(\mathbf{k}_t; tt_2) G_{mn}^<(\mathbf{k}_t; t_2 t) + \Sigma_{nm}^<(\mathbf{k}_t; tt_2) G_{mn}^A(\mathbf{k}_t; t_2 t)] - \right. \\
&\quad \left. \underbrace{[G_{nm}^R(\mathbf{k}_t; tt_2) \Sigma_{mn}^<(\mathbf{k}_t; t_2 t) + G_{nm}^<(\mathbf{k}_t; tt_2) \Sigma_{mn}^A(\mathbf{k}_t; t_2 t)]}_{=0, \text{ because of condition (G.6)}} \right) \} \\
&= -\frac{J_n(t) - J_{n-1}(t)}{\Delta}. \tag{2.93}
\end{aligned}$$

It is important to note that the boundary conditions are not included in the self-energies but the index m takes into account points from the device and from the leads. The next step consists in separating J_n from J_{n-1} by decomposing equation (2.93). Caroli proposed an useful ansatz in [6]. The current J at a point between $n - 1$ and n (called J_n for simplicity) is the difference between the flow of particles from left to right and from right to left. Thus on operator J of the form

$$\begin{aligned}
J_n(t) &\propto \sum_{l \geq n+1} \sum_{m \leq n} T_{lm} \langle a_l^\dagger a_m \rangle - \sum_{l \leq n} \sum_{m \geq n+1} T_{lm} \langle a_l^\dagger a_m \rangle \\
&\propto \sum_{l \geq n+1} \sum_{m \leq n} \left(T_{lm} \langle a_l^\dagger a_m \rangle - \langle a_m^\dagger a_l \rangle T_{ml} \right) \tag{2.94}
\end{aligned}$$

is expected. This leads to the following expression for the current $J_n(t)$, valid for stationary and non-stationary cases, even when scattering mechanisms are present

$$J_n(t) = -\frac{e}{A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{\mathbf{k}_t, \sigma} (h_{lm} G_{ml}^<(\mathbf{k}_t; tt) - G_{lm}^<(\mathbf{k}_t; tt) h_{ml}) \tag{2.95}$$

and as it can easily be shown, this expression in combination with the one for J_{n-1} satisfies equation (2.93).

For stationary situations, the current is the same everywhere in a device and one can choose the place where it is computed. Therefore, assuming that the device contacts are in equilibrium and that no scattering occurs between any contacts and the active part of the device, the current can be evaluated at the interface between a contact and the active region. This means that the index m corresponds to points in the contact and l to points in the active region. With the help of (2.44), equation

(2.95) reduces to

$$\begin{aligned}
J_n &= -\frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} (h_{lm} G_{ml}^<(\mathbf{k}_t; E) - G_{lm}^<(\mathbf{k}_t; E) h_{ml}) \\
&= -\frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} 2\text{Re} \{ h_{lm} G_{ml}^<(\mathbf{k}_t; E) \}.
\end{aligned} \tag{2.96}$$

The second line is obtained with the help of equation (2.45). The boundary conditions from section 2.6 allow a simplification for $G_{ml}^<(\mathbf{k}_t; E)$, where m belongs to any point of the device contacts with Fermi distribution of the carriers, l to the active part of the device, and n is at the interface between both regions. $U_{LC,CL}$ in equation (2.87) corresponds to h_{ml,l_m} . Hence, one obtains for the lesser Green's function

$$\begin{aligned}
G_{ml}^<(\mathbf{k}_t; E) &= \sum_{l_1 \geq n+1} \sum_{m_1 \leq n} (g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) \\
&\quad + g_{mm_1}^R(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^<(\mathbf{k}_t; E))
\end{aligned} \tag{2.97}$$

and for the current density

$$\begin{aligned}
J_n &= -\frac{e}{\hbar A} \sum_{\substack{l \geq n+1 \\ m \leq n}} \sum_{\substack{l_1 \geq n+1 \\ m_1 \leq n}} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \overbrace{(2\text{Re} \{ h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) \}}^{J_{lmm_1 l_1}^{p1}(k_t; E)} \\
&\quad + \underbrace{2\text{Re} \{ h_{lm} g_{mm_1}^R(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^<(\mathbf{k}_t; E) \}}_{J_{lmm_1 l_1}^{p2}(k_t; E)})
\end{aligned} \tag{2.98}$$

Under the assumption that the contacts are in equilibrium, equation (2.98) can be further simplified. One starts with the first line of (2.98): because of the Fermi distribution in the contacts, the fluctuation-dissipation theorem from section 1.3.3 can be applied for $g_{mm_1}^<$. This leads to the following expression (see eq. (1.31))

$$g_{mm_1}^<(\mathbf{k}_t; E) = i f^{Cont}(E) A_{mm_1}(\mathbf{k}_t; E), \tag{2.99}$$

where $f^{Cont}(E)$ represents the Fermi-distribution function of the considered contact. The first line can then be rewritten as

$$\begin{aligned}
2\text{Re} \{ h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) \} &= J_{lmm_1 l_1}^{p1}(\mathbf{k}_t; E) \\
&= h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) + \\
&\quad (h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E))^\dagger \\
&= h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) +
\end{aligned}$$

$$\begin{aligned}
& h_{lm}^\dagger [g_{mm_1}^<(\mathbf{k}_t; E)]^\dagger h_{m_1 l_1}^\dagger [G_{l_1 l}^A(\mathbf{k}_t; E)]^\dagger \\
&= h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) - \\
& h_{ml} g_{m_1 m}^<(\mathbf{k}_t; E) h_{l_1 m_1} G_{ll_1}^R(\mathbf{k}_t; E) \quad (2.100)
\end{aligned}$$

The third equality is derived from the properties of the Green's functions described in equation (2.45). It is important to note that the sum over the index m ($\sum_{m \leq n}$) is the same as the sum over m_1 ($\sum_{m_1 \leq n}$). The same holds for the sum over l and l_1 . As consequence, m can be replaced by m_1 , m_1 by m , l by l_1 , and l_1 by l in the last line of (2.100). This yields

$$\begin{aligned}
J_{lmm_1 l_1}^{p1}(\mathbf{k}_t; E) &= h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^A(\mathbf{k}_t; E) - \\
& h_{m_1 l_1} g_{mm_1}^<(\mathbf{k}_t; E) h_{lm} G_{l_1 l}^R(\mathbf{k}_t; E) \\
&= -h_{lm} g_{mm_1}^<(\mathbf{k}_t; E) h_{m_1 l_1} (G_{l_1 l}^R(\mathbf{k}_t; E) - G_{l_1 l}^A(\mathbf{k}_t; E)) \\
&= -f^{Cont}(E) h_{lm} A_{mm_1}(\mathbf{k}_t; E) h_{m_1 l_1} i (G_{l_1 l}^R(\mathbf{k}_t; E) - G_{l_1 l}^A(\mathbf{k}_t; E)) \\
&= -f^{Cont}(E) h_{lm} A_{mm_1}(\mathbf{k}_t; E) h_{m_1 l_1} A_{l_1 l}(\mathbf{k}_t; E). \quad (2.101)
\end{aligned}$$

The same argumentation is also applied to the second part of equation (2.98) $J_{lmm_1 l_1}^{p2}(k_t; E)$ with the following result

$$\begin{aligned}
J_{lmm_1 l_1}^{p2}(\mathbf{k}_t; E) &= 2\text{Re} \{ h_{lm} g_{mm_1}^R(\mathbf{k}_t; E) h_{m_1 l_1} G_{l_1 l}^<(\mathbf{k}_t; E) \} \\
&= -h_{lm} A_{mm_1}(\mathbf{k}_t; E) h_{m_1 l_1} i G_{l_1 l}^<(\mathbf{k}_t; E) \quad (2.102)
\end{aligned}$$

It remains to insert equations (2.101) and (2.102) into the expression for the current density (2.98)

$$J_n = \frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{l_1 \geq n+1} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \Gamma_{ll_1}^{Cont}(\mathbf{k}_t; E) \left(f^{Cont}(E) A_{l_1 l}(\mathbf{k}_t; E) + i G_{l_1 l}^<(\mathbf{k}_t; E) \right)$$

(2.103)

with

$$\Gamma_{ll_1}^{Cont}(\mathbf{k}_t; E) = \sum_{m \leq n} \sum_{m_1 \leq n} h_{lm} A_{mm_1}(\mathbf{k}_t; E) h_{m_1 l_1}. \quad (2.104)$$

Equation (2.103) corresponds to equation (5) of [8] and as the authors note, it is valid even when scattering processes and many-body interactions are present in the active part of the device. The only assumption is that the self-energies between contacts and active region vanish.

2.7.1 2-Contact Device

One considers now a device with two different contacts L and R on the left and the right side of a central active region, respectively, discretized with N points. The current flowing from the left contact inside the device is given by equation (2.103)

$$J_L = \frac{e}{\hbar A} \sum_{l=1}^N \sum_{l_1=1}^N \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \Gamma_{ll_1}^L(\mathbf{k}_t; E) (f^L(E) A_{l_1 l}(\mathbf{k}_t; E) + i G_{l_1 l}^<(\mathbf{k}_t; E)).$$

The current flowing from the central part of the device to the right contact $J_R(t)$ is calculated as $J_L(t)$ but gets a minus sign because the active region (and therefore the index l) is situated on the left side of contact R . As consequence, l in equation (2.103) must be smaller than $n - 1$ and this causes the minus sign (eq. (2.103) describes the current flowing from one reservoir into the device. The relative position of each other must be taken into account and is contained in the minus sign of J_R)

$$J_R = -\frac{e}{\hbar A} \sum_{l=1}^N \sum_{l_1=1}^N \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \Gamma_{ll_1}^R(\mathbf{k}_t; E) (f^R(E) A_{l_1 l}(\mathbf{k}_t; E) + i G_{l_1 l}^<(\mathbf{k}_t; E)).$$

The index R in $\Gamma_{ll_1}^R$ and $f^R(E)$ indicates the right contact and must not be confused with “retarded” like in G^R . Because the current flowing inside the device J_L must be the same as the one flowing outside J_R for a stationary regime, equation (2.103) can be symmetrized

$$\begin{aligned} J &= \left(\frac{J_L + J_R}{2} \right) \\ &= \frac{e}{2\hbar A} \sum_{l=1}^N \sum_{l_1=1}^N \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \left\{ (\Gamma_{ll_1}^L(\mathbf{k}_t; E) f^L(E) - \Gamma_{ll_1}^R(\mathbf{k}_t; E) f^R(E)) A_{l_1 l}(\mathbf{k}_t; E) \right. \\ &\quad \left. + i (\Gamma_{ll_1}^L(E) - \Gamma_{ll_1}^R(E)) G_{l_1 l}^<(\mathbf{k}_t; E) \right\}. \end{aligned}$$

2.7.2 Non-Interacting Device (Ballistic Transport)

Keeping the same device as before, but assuming that no interaction occurs in the central active region, equation (2.103) can be simplified by expressing the spectral function $A_{l_1 l}(\mathbf{k}_t; E)$ and the lesser Green's function $G_{l_1 l}^<(\mathbf{k}_t; E)$ with the help of the boundary conditions described in section 2.6. After some algebra, one obtains

$$G_{l_1 l}^< = \sum_{l_2, l_3} \left(\sum_{m_1, m_2} G_{l_1 l_2}^R h_{l_2 m_1} g_{m_1 m_2}^< h_{m_2 l_3} G_{l_3 l}^A + \sum_{m_3, m_4} G_{l_1 l_2}^R h_{l_2 m_3} g_{m_3 m_4}^< h_{m_4 l_3} G_{l_3 l}^A \right),$$

where the indices l_2 and l_3 belong to the non-interacting active part of the device, m_1 and m_2 to the left contact, and m_3 and m_4 to the right contact. $g_{m_1 m_2}^<$ and $g_{m_3 m_4}^<$ represent the carrier distribution within the equilibrated contacts, which enables the

use of the fluctuation-dissipation theorem of section 1.3.3. Furthermore, recalling the definition (2.104) leads to the following equations

$$\begin{aligned} \sum_{m_1, m_2} h_{l_2 m_1} g_{m_1 m_2}^< h_{m_2 l_3} &= \sum_{m_1, m_2} i f^L h_{l_2 m_1} A_{m_1 m_2} h_{m_2 l_3} \\ &= i f^L \Gamma_{l_2 l_3}^L \\ \sum_{m_3, m_4} h_{l_2 m_3} g_{m_3 m_4}^< h_{m_4 l_3} &= \sum_{m_3, m_4} i f^R h_{l_2 m_3} A_{m_3 m_4} h_{m_4 l_3} \\ &= i f^R \Gamma_{l_2 l_3}^R \end{aligned}$$

and as consequence

$$G_{l_1 l}^< = \sum_{l_2, l_3} i G_{l_1 l_2}^R (f^L \Gamma_{l_2 l_3}^L + f^R \Gamma_{l_2 l_3}^R) G_{l_3 l}^A. \quad (2.105)$$

Similarly, for the spectral function $A_{l_1 l}$, one obtains

$$\begin{aligned} A_{l_1 l} &= i (G_{l_1 l}^> - G_{l_1 l}^<) \\ &= \sum_{l_2, l_3} \left(\sum_{m_1, m_2} G_{l_1 l_2}^R h_{l_2 m_1} A_{m_1 m_2} h_{m_2 l_3} G_{l_3 l}^A \right. \\ &\quad \left. + \sum_{m_3, m_4} G_{l_1 l_2}^R h_{l_2 m_3} A_{m_3 m_4} h_{m_4 l_3} G_{l_3 l}^A \right) \\ &= \sum_{l_2, l_3} G_{l_1 l_2}^R (\Gamma_{l_2 l_3}^L + \Gamma_{l_2 l_3}^R) G_{l_3 l}^A. \end{aligned} \quad (2.106)$$

The insertion of equations (2.105) and (2.106) into (2.103) yields the usual two-terminal Landauer formula for the non-interacting case

$$J = \frac{e}{\hbar A} \sum_{ll_1} \sum_{l_2 l_3} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} [\Gamma_{ll_1}^L G_{l_1 l_2}^R \Gamma_{l_2 l_3}^R G_{l_3 l}^A] (\mathbf{k}_t; E) (f^L(E) - f^R(E)), \quad (2.107)$$

where the indices l, l_1, l_2, l_3 run over all the points within the non-interacting active part of the device.

2.7.3 Interacting Device

One considers a device with non-interacting leads/contacts and an interacting central part. The starting point remains equation (2.103) but for interaction in the central part of the device, one obtains a different expression for $G_{l_1 l}^<$ and $A_{l_1 l}$

$$\begin{aligned} G_{l_1 l}^< &= \sum_{l_2, l_3} G_{l_1 l_2}^R (i f^L \Gamma_{l_2 l_3}^L + i f^R \Gamma_{l_2 l_3}^R + \Sigma_{l_2 l_3}^<) G_{l_3 l}^A \\ A_{l_1 l} &= \sum_{l_2, l_3} G_{l_1 l_2}^R (\Gamma_{l_2 l_3}^L + \Gamma_{l_2 l_3}^R + i (\Sigma_{l_2 l_3}^> - \Sigma_{l_2 l_3}^<)) G_{l_3 l}^A. \end{aligned} \quad (2.108)$$

The interactions like carrier-phonon scattering are cast into the self-energies $\Sigma_{l_2 l_3}^<$ and $\Sigma_{l_2 l_3}^>$. The new equations (2.108) for the Green's function $G_{l_1 l}^<$ and for the spectral function $A_{l_1 l}$ cause a two-part current density J

$$J = J_{coh} + J_{in}, \quad (2.109)$$

where J_{coh} is given by equation (2.107), but its value is different from the one in the previous section because $G_{l_1 l_2}^R$ and $G_{l_3 l}^A$ are calculated in the presence of interaction. The evaluation of J_{in} yields

$$\begin{aligned} J_{in} &= \frac{ie}{\hbar A} \sum_{ll_1} \sum_{l_2 l_3} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \Gamma_{ll_1}^L(\mathbf{k}_t; E) G_{l_1 l_2}^R(\mathbf{k}_t; E) \{ \Sigma_{l_2 l_3}^>(\mathbf{k}_t; E) f^L(E) \\ &\quad + \Sigma_{l_2 l_3}^<(\mathbf{k}_t; E) (1 - f^L(E)) \} G_{l_3 l}^A(\mathbf{k}_t; E) \\ &= \frac{ie}{\hbar A} \sum_{ll_1 l_2 l_3} \sum_{m_1 m_2} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} h_{lm_1} A_{m_1 m_2}(\mathbf{k}_t; E) h_{m_2 l_1} G_{l_1 l_2}^R(\mathbf{k}_t; E) G_{l_3 l}^A(\mathbf{k}_t; E) \\ &\quad \times \{ \Sigma_{l_2 l_3}^>(\mathbf{k}_t; E) i f^L(E) + \Sigma_{l_2 l_3}^<(\mathbf{k}_t; E) i (1 - f^L(E)) \} \\ &= \frac{e}{\hbar A} \sum_{ll_1 l_2 l_3} \sum_{m_1 m_2} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} h_{lm_1} h_{m_2 l_1} G_{l_1 l_2}^R(\mathbf{k}_t; E) G_{l_3 l}^A(\mathbf{k}_t; E) \\ &\quad \times \{ \Sigma_{l_2 l_3}^>(\mathbf{k}_t; E) g_{m_1 m_2}^<(\mathbf{k}_t; E) - \Sigma_{l_2 l_3}^<(\mathbf{k}_t; E) g_{m_1 m_2}^>(\mathbf{k}_t; E) \}, \end{aligned} \quad (2.110)$$

where the indices l, l_1, l_2, l_3 run over all the points within the interacting central part of the device and m_1, m_2 are situated in the left contact/lead. The last equality in (2.110) is obtained from the fluctuation-dissipation theorem (section 1.3.3).

2.7.4 Büttiker Probes

To compute current when scattering events are present requires the knowledge of the self-energies $\Sigma^>$ and $\Sigma^<$. Because it is very difficult to obtain them self-consistently with the Green's functions, a simpler way to take into account scattering is of great interest. The idea is to approximate the retarded self-energies by a phenomenological decay time τ which can be energy-dependent or not. This gives for the retarded self-energy $\Sigma_{nm}^R(\mathbf{k}_t; E)$ (unit [eV]) assuming that it is only diagonal

$$\Sigma_{nm}^R(\mathbf{k}_t; E) = -i \frac{\hbar}{\tau} \delta_{nm}. \quad (2.111)$$

Because of the current condition presented in Appendix G, the lesser self-energy $\Sigma_{nm}^<(\mathbf{k}_t; E)$ cannot be chosen without restriction, but must be diagonal and must

fulfill

$$\sum_{\mathbf{k}_t} \int dE \left(\Sigma_{nn}^R(\mathbf{k}_t; E) G_{nn}^<(\mathbf{k}_t; E) + \Sigma_{nn}^<(\mathbf{k}_t; E) G_{nn}^A(\mathbf{k}_t; E) - G_{nn}^R(\mathbf{k}_t; E) \Sigma_{nn}^<(\mathbf{k}_t; E) - G_{nn}^<(\mathbf{k}_t; E) \Sigma_{nn}^A(\mathbf{k}_t; E) \right) = 0. \quad (2.112)$$

At equilibrium, as in the reservoirs, there is a relation between the retarded and lesser Green's functions/self-energies due to the fluctuation dissipation theorem of section 1.3.3

$$\begin{aligned} G_{nn}^<(\mathbf{k}_t; E) &= i f(E) A_{nn}(\mathbf{k}_t; E), & A_{nn}(\mathbf{k}_t; E) &= i (G_{nn}^R(\mathbf{k}_t; E) - G_{nn}^A(\mathbf{k}_t; E)), \\ \Sigma_{nn}^<(\mathbf{k}_t; E) &= i f(E) \Gamma_{nn}(\mathbf{k}_t; E), & \Gamma_{nn}(\mathbf{k}_t; E) &= i (\Sigma_{nn}^R(\mathbf{k}_t; E) - \Sigma_{nn}^A(\mathbf{k}_t; E)). \end{aligned}$$

$f(E)$ is the Fermi distribution of the electrons for energy E . All these equilibrium conditions can now be applied to determine the lesser self-energies from the retarded one given in equation (2.111). This yields

$$\begin{aligned} \Sigma_{nn}^<(\mathbf{k}_t; E) &= i f_n(E) \Gamma_{nn}(\mathbf{k}_t; E) \\ &= 2i f_n(E) \frac{\hbar}{\tau}. \end{aligned} \quad (2.113)$$

Taking this into account, with some simple algebra and previously defined relations for the Green's functions, condition (2.112) becomes

$$\begin{aligned} &\sum_{\mathbf{k}_t} \int dE \left(G_{nn}^<(\mathbf{k}_t; E) (\Sigma_{nn}^R(\mathbf{k}_t; E) - \Sigma_{nn}^A(\mathbf{k}_t; E)) - \Sigma_{nn}^<(\mathbf{k}_t; E) (G_{nn}^R(\mathbf{k}_t; E) - G_{nn}^A(\mathbf{k}_t; E)) \right) = \\ &\sum_{\mathbf{k}_t} \int dE \left(G_{nn}^<(\mathbf{k}_t; E) \Sigma_{nn}^>(\mathbf{k}_t; E) - \Sigma_{nn}^<(\mathbf{k}_t; E) G_{nn}^>(\mathbf{k}_t; E) \right) = \\ &\sum_{\mathbf{k}_t, m} \int dE \left(G_{nm}^R(\mathbf{k}_t; E) \underbrace{\Sigma_{mm}^<(\mathbf{k}_t; E)}_{i f_m(E) \Gamma_{mm}(\mathbf{k}_t; E)} G_{mn}^A(\mathbf{k}_t; E) \underbrace{\Sigma_{nn}^>(\mathbf{k}_t; E)}_{i (f_n(E) - 1) \Gamma_{nn}(\mathbf{k}_t; E)} - \right. \\ &\quad \left. \underbrace{\Sigma_{nn}^<(\mathbf{k}_t; E)}_{i f_n(E) \Gamma_{nn}(\mathbf{k}_t; E)} G_{nm}^R(\mathbf{k}_t; E) \underbrace{\Sigma_{mm}^>(\mathbf{k}_t; E)}_{i (f_m(E) - 1) \Gamma_{mm}(\mathbf{k}_t; E)} G_{mn}^A(\mathbf{k}_t; E) \right) = \\ &\sum_{\mathbf{k}_t, m} \int dE T^{nm}(\mathbf{k}_t; E) (f_m(E) - f_n(E)) = 0 \end{aligned} \quad (2.114)$$

with

$$T^{nm}(\mathbf{k}_t; E) = \Gamma_{nn}(\mathbf{k}_t; E) G_{nm}^R(\mathbf{k}_t; E) \Gamma_{mm}(\mathbf{k}_t; E) G_{mn}^A(\mathbf{k}_t; E). \quad (2.115)$$

$T^{nm}(\mathbf{k}_t; E)$ is the transmission from point n to point m where m covers all the discretization points and n only the ones where scattering events occur, i.e. not the

boundary condition points.

The current condition (2.114) as obtained by the use of the quasi-equilibrium approximation for the self-energies, is valid for each point n where scatterings are present. If there are N points, this implies that N free parameters must be present: they will be the Fermi level at each point, which are no more physical parameters but mathematical tricks to keep the current constant along the device. The replacement of the self-consistent self-energies by a phenomenological decay time for the retarded ones as well as the application of the equilibrium condition for the lesser ones is equivalent to the use of Büttiker probes as scattering centers [17].

2.7.4.1 Current Calculation with Büttiker Probes

The current density J_n at position z_n is given by equation (2.96) when scattering mechanisms are present or not. Because of the form of the Hamiltonian parts h_{lm} , as described in the next chapter, the equation for J_n becomes

$$J_n = -\frac{e}{\hbar A} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} (h_{n+1n} G_{nn+1}^<(\mathbf{k}_t; E) - G_{n+1n}^<(\mathbf{k}_t; E) h_{nn+1}). \quad (2.116)$$

The goal is now to make the Fermi distribution functions appear in equation (2.116) in order to obtain an expression similar to the ballistic case (2.107). First of all, the boundary conditions from section 2.6 are used: the point $n+1$ will belong to the central part of the device and the other remaining points are assumed parts of the leads. As in section 2.6, the small Green's functions $g(\mathbf{k}_t; E)$ come from the leads (all the points except $n+1$) and the big ones $G(\mathbf{k}_t; E)$ from the device. The variables \mathbf{k}_t and E are neglected if they do not contribute to the signification of the equation. This leads to

$$\begin{aligned} G_{nn+1}^<(\equiv G_{LC}^<) &= g_{nn}^< h_{nn+1} G_{n+1n+1}^A + g_{nn}^R h_{nn+1} G_{n+1n+1}^< \\ G_{n+1n}^<(\equiv G_{CL}^<) &= G_{n+1n+1}^< h_{n+1n} g_{nn}^A + G_{n+1n+1}^R h_{n+1n} g_{nn}^< \end{aligned} \quad (2.117)$$

and therefore

$$\begin{aligned} h_{n+1n} G_{nn+1}^< - G_{n+1n}^< h_{nn+1} &= h_{n+1n} g_{nn}^< h_{nn+1} \underbrace{\left(G_{n+1n+1}^A - G_{n+1n+1}^R \right)}_{G_{n+1n+1}^< - G_{n+1n+1}^>} + \\ &\quad h_{n+1n} \underbrace{\left(g_{nn}^R - g_{nn}^A \right)}_{g_{nn}^> - g_{nn}^<} h_{nn+1} G_{n+1n+1}^< \\ &= h_{n+1n} g_{nn}^> h_{nn+1} G_{n+1n+1}^< - h_{n+1n} g_{nn}^< h_{nn+1} G_{n+1n+1}^>. \end{aligned} \quad (2.118)$$

To close the equation, one has to find an expression for g and G as function of the Büttiker self-energies. This is done with

$$g_{nn}^{<, >} = \sum_{m_1 < n+1} g_{nm_1}^R \Sigma_{m_1 m_1}^{<, >} g_{m_1 n}^A,$$

$$\begin{aligned}
G_{n+1n+1}^{<,>} &= G_{n+1n+1}^R h_{n+1n} g_{nn}^{<,>} h_{nn+1} G_{n+1n+1}^A + \\
&\quad G_{n+1n+1}^R h_{n+1n+2} g_{n+2n+2}^{<,>} h_{n+2n+1} G_{n+1n+1}^A + \\
&\quad G_{n+1n+1}^R \Sigma_{n+1n+1}^{<,>} G_{n+1n+1}^A, \\
g_{n+2n+2}^{<,>} &= \sum_{m_2 > n+1} g_{nm_2}^R \Sigma_{m_2 m_2}^{<,>} g_{m_2 n}^A.
\end{aligned} \tag{2.119}$$

Inserting these results into the last line of equation (2.118) yields

$$\begin{aligned}
&h_{n+1n} g_{nn}^{>} h_{nn+1} G_{n+1n+1}^{<} - h_{n+1n} g_{nn}^{<} h_{nn+1} G_{n+1n+1}^{>} = \\
&h_{n+1n} g_{nn}^{>} h_{nn+1} G_{n+1n+1}^R h_{n+1n+2} g_{n+2n+2}^{<} h_{n+2n+1} G_{n+1n+1}^A - \\
&h_{n+1n} g_{nn}^{<} h_{nn+1} G_{n+1n+1}^R h_{n+1n+2} g_{n+2n+2}^{>} h_{n+2n+1} G_{n+1n+1}^A + \\
&G_{n+1n+1}^R h_{n+1n} h_{nn+1} G_{n+1n+1}^A \left(g_{nn}^{>} \Sigma_{n+1n+1}^{<} - g_{nn}^{<} \Sigma_{n+1n+1}^{>} \right) = \\
&\sum_{m_1 < n+1} \sum_{m_2 > n+1} h_{n+1n} g_{nm_1}^R g_{m_1 n}^A h_{nn+1} G_{n+1n+1}^R h_{n+1n+2} g_{n+2m_2}^R g_{m_2 n+2}^A \\
&\quad h_{n+2n+1} G_{n+1n+1}^A \left(\Sigma_{m_1 m_1}^{>} \Sigma_{m_2 m_2}^{<} - \Sigma_{m_1 m_1}^{<} \Sigma_{m_2 m_2}^{>} \right) + \\
&\sum_{m_1 < n+1} G_{n+1n+1}^R h_{n+1n} g_{nm_1}^R g_{m_1 n}^A h_{nn+1} G_{n+1n+1}^A \left(\Sigma_{m_1 m_1}^{>} \Sigma_{n+1n+1}^{<} - \right. \\
&\quad \left. \Sigma_{m_1 m_1}^{<} \Sigma_{n+1n+1}^{>} \right).
\end{aligned} \tag{2.120}$$

From the boundary conditions of section 2.6, it is known that

$$\begin{aligned}
G_{LL}^R &= g_{LL}^R \left(1 + U_{LC} G_{CL}^R \right) \\
&= g_{LL}^R \left(1 + U_{LC} G_{CC}^R U_{CL} g_{LL}^R \right) \\
G_{LC}^R &= g_{LL}^R U_{LC} G_{CC}^R
\end{aligned} \tag{2.121}$$

so that one has

$$\begin{aligned}
G_{m_1 m_2}^R &= g_{m_1 n}^R h_{nn+1} G_{n+1n+1}^R h_{n+1n+2} g_{n+2m_2}^R \\
G_{m_1 n+1}^R &= g_{m+1n}^R h_{nn+1} G_{n+1n+1}^R.
\end{aligned} \tag{2.122}$$

To obtain these results, the fact that $g_{m_1 m_2}^R = 0$ is taken into account: this comes from the definition of the lead Green's function g^R which are calculated when $h_{nn+1} = h_{n+1n+2} = 0$. Furthermore, due to the form of the Green's functions equation, one has the following property

$$g_{m_1 n}^R = g_{nm_1}^R, \text{ because } \left((g^R)^{-1} \right)^* = \left((g^R)^{-1} \right)^T. \tag{2.123}$$

This is only valid for an homogeneous space discretization. With the help of equations (2.122) and (2.123), the expression (2.120) can be further simplified and one

obtains for the current density $J_{n+\frac{1}{2}}$ (one also needs to rewrite the self-energies as derived in (2.113))

$$J_{n+\frac{1}{2}} = -\frac{e}{A\hbar} \sum_{\mathbf{k}\mathbf{t}\sigma} \sum_{m_1 < n+1} \sum_{m_2 \geq n+1} \int dE \underbrace{[\Gamma_{m_1 m_1} G_{m_1 m_2}^R \Gamma_{m_2 m_2} G_{m_2 m_1}^A]}_{T^{m_1 m_2}(\mathbf{k}\mathbf{t}; E)} (\mathbf{k}\mathbf{t}; E) (f_{m_2}(E) - f_{m_1}(E)). \quad (2.124)$$

If one evaluates now $J_{n-\frac{1}{2}}$ and builds the divergence of the current density J , one can easily prove that it disappears and that the current is therefore constant over the device.

Chapter 3

Applications

In this section, four different approaches to solve Quantum Transport problems with Green's functions are presented:

3.1 Resonant Tunneling Based Quantum Devices

This application is based on the paper of Roger Lake and al. [4] and describes the simulation of resonant tunneling based quantum devices (fig. 3.1). Their design requires accurate modeling of the quantum charge, resonant levels, and scattering effects for complicated 1-D potential profile made possible by hetero-epitaxial growth. Nonequilibrium Green's functions theory is formulated to meet these three main challenges.

3.1.1 Model Summary

First of all, the structure to simulate is discretized with N points for the active device (central part of figure 3.1) going from 1 to N , N_L for the left reservoir (emitter) going from $-N_L + 1$ to 0, and N_R for the right one (collector) going from $N + 1$ to $N + N_R$. The potential in the reservoirs does not need to be constant and can be large: it is no more necessary to inject carriers from the flat band region of the contacts. This approach is based on Dyson's equation treatment of the contacts developed by Caroli in [6].

Furthermore, the effects of the scattering mechanisms (optical (H_{opp}) and acoustic phonon (H_{acp}) scattering, alloy scattering (H_{al}), interface roughness scattering (H_{ir}), and ionized dopant scattering (H_{id})) are treated as perturbation via Σ while the effects of the contacts are taken into account exactly through a boundary self-energy Σ^B .

All these effects are included in the Hamiltonian given by

$$H = H_0 + \underbrace{H_{opp} + H_{acp} + H_{ir} + H_{al} + H_{id}}_{\Sigma} \quad (3.1)$$

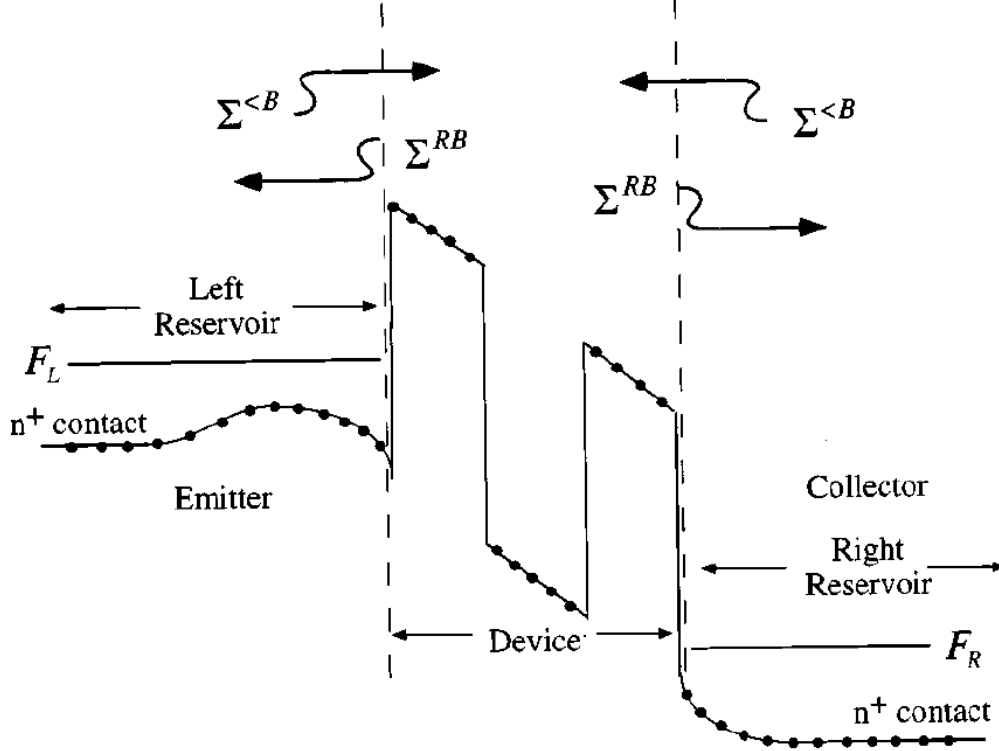


Figure 3.1: Resonant tunneling quantum device. The structure is partitioned into two large reservoirs, with Fermi distribution and a short device.

where H_0 is broken down into five parts, the device (H^D), the left (H^L) and right contacts (H^R), and the tunnel Hamiltonian between the device and the left/right contact (H^{DL} and H^{DR})

$$H_0 = H_0^D + \underbrace{H_0^L + H_0^R + H_0^{DL} + H_0^{DR}}_{\Sigma^B}. \quad (3.2)$$

The required eigenfunctions to expand the Green's functions, as in section 2.4, are cation and anion orbitals situated around one of the N layers of the device corresponding to the lattice points. For example, in the sp^3 model, there are 1 s and 3 p orbitals neglecting spin and in the single tight-binding model which will be used for the rest of the section, there is only one orbital per layer (the anion and cation are lumped into a single orbital). In this case, one can imagine the orbital as a pseudo-Wannier function centered around a lattice point. H_0 is given by

$$H_0 = -\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + \frac{\hbar^2 k_t^2}{2m^*} + V(z) \quad (3.3)$$

and as consequence, h_{nm} from equation (2.45) becomes

$$h_{nm} = \int dz \phi_n^*(z) H_0 \phi_m(z) = \begin{cases} D_n(k_t) = \frac{\hbar^2}{2\Delta^2} \left(\frac{1}{m^-} + \frac{1}{m^+} \right) + V_n + \frac{\hbar^2 k_t^2}{2m^*} & m = n \\ -t_{nm} = -\frac{\hbar^2}{(m_n^* + m_m^*)\Delta^2} & m = n \pm 1 \\ 0 & \text{otherwise,} \end{cases}$$

where $m_- = (m_n^* + m_{n-1}^*)/2$, $m_+ = (m_n^* + m_{n+1}^*)/2$, $\Delta = z_n - z_{n-1}$, and $V_n = V(z_n)$ (1D Potential with Hartree correction). To prove these equalities, one starts from the eigenfunction expansion of $G(x_1 t_1; x_2 t_2)$ given in equations (2.25), (2.26) and the result (2.34) so that one obtains (with a position-independent effective mass m^*)

$$\begin{aligned} \sum_l h_{nl} G_{lm}^<(\mathbf{k}_t; t_1 t_2) &= \\ \int dz_1 \int dz_2 \phi_n^*(z_1) \left(-\frac{\hbar^2}{2m^*} \nabla_{z_1}^2 + V(z_1) + \frac{\hbar^2 \mathbf{k}_t^2}{2m^*} \right) G(\mathbf{k}_t; z_1 t_1; z_2 t_2) \phi_m(z_2) &= \\ \int dz_1 \phi_n^*(z_1) \left[\left(\frac{\hbar^2}{m^* \Delta^2} + V(z_1) + \frac{\hbar^2 \mathbf{k}_t^2}{2m^*} \right) G_m(\mathbf{k}_t; z_1; t_1 t_2) - \right. \\ \left. \frac{\hbar^2}{2m^* \Delta^2} (G_m(\mathbf{k}_t; z_1 + \Delta; t_1 t_2) + G_m(\mathbf{k}_t; z_1 - \Delta; t_1 t_2)) \right] &= \quad (3.4) \\ \sum_{n_1} \int dz_1 \phi_n^*(z_1) \left[\left(\frac{\hbar^2}{m^* \Delta^2} + V(z_1) + \frac{\hbar^2 \mathbf{k}_t^2}{2m^*} \right) G_{n_1 m}(\mathbf{k}_t; t_1 t_2) - \right. \\ \left. \frac{\hbar^2}{2m^* \Delta^2} (G_{n_1+1 m}(\mathbf{k}_t; t_1 t_2) + G_{n_1-1 m}(\mathbf{k}_t; t_1 t_2)) \right] \phi_{n_1}(z_1) &= \\ D_n G_{nm}(\mathbf{k}_t; t_1 t_2) - t_{nn+1} G_{n+1 m}(\mathbf{k}_t; t_1 t_2) - t_{nn-1} G_{n-1 m}(\mathbf{k}_t; t_1 t_2). \end{aligned}$$

For completeness, one derives the expressions for the boundary self-energies, where the effects of the contacts on the device using Dyson's equations are included exactly. For that purpose, one refers to the boundary conditions described in section 2.6 with the same assumptions as there. In the single-band tight-binding model, U_{LC} (lead-center) and U_{CL} (center-lead) have only two possible values

$$U_{LC} = t_{01}, \quad t_{N+1N} \quad \text{and} \quad U_{CL} = t_{10}, \quad t_{NN+1}. \quad (3.5)$$

If i and j are two points in the device between 1 and N , one obtains with Eq. (2.82)

$$G_{ij}^R = g_{ij}^R + g_{i1}^R \underbrace{(-t_{10}) g_{00}^R (-t_{01})}_{\Sigma_{11}^{RB}} G_{1j}^R + g_{iN}^R \underbrace{(-t_{NN+1}) g_{N+1N+1}^R (-t_{N+1N})}_{\Sigma_{NN}^{RB}} G_{Nj}^R. \quad (3.6)$$

The G 's are exact Green's functions while the g 's are Green's functions when contacts and device are not coupled, i.e. t_{10} , t_{01} , t_{NN+1} , and t_{N+1N} are set to zero. For instance, g_{ij}^R obeys the following equation, combination of (2.45) and (2.83)

$$\sum_{l \in N} \underbrace{[(E - D_i) \delta_{il} + t_{il} - \Sigma_{il}^R]}_{[g_{il}^R]^{-1}} g_{lj}^R = \delta_{ij}. \quad (3.7)$$

Operating with $[g_{il}^R]^{-1}$ on G_{lj}^R from equation (3.6) and summing over l yields

$$\sum_{l \in N} [(E - D_i) \delta_{il} + t_{il} - \Sigma_{il}^R] G_{lj}^R = \delta_{ij} + \delta_{i1} \Sigma_{11}^{RB} G_{1j}^R + \delta_{iN} \Sigma_{NN}^{RB} G_{Nj}^R \quad (3.8)$$

This equation can be rewritten in matrix form as follows

$$[G^R] = \begin{pmatrix} E - D_1 - \Sigma_{11}^{RB} - \Sigma_{11}^R & t_{12} - \Sigma_{12}^R & -\Sigma_{13}^R & \cdots & -\Sigma_{1N-1}^R & -\Sigma_{1N}^R \\ t_{21} - \Sigma_{21}^R & E - D_2 - \Sigma_{22}^R & t_{23} - \Sigma_{23}^R & \cdots & -\Sigma_{2N-1}^R & -\Sigma_{2N}^R \\ -\Sigma_{31}^R & t_{32} - \Sigma_{32}^R & E - D_3 - \Sigma_{33}^R & \cdots & -\Sigma_{3N-1}^R & -\Sigma_{3N}^R \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\Sigma_{N-11}^R & -\Sigma_{N-12}^R & -\Sigma_{N-13}^R & \cdots & E - D_{N-1} - \Sigma_{N-1N-1}^R & t_{N-1N} - \Sigma_{N-1N}^R \\ -\Sigma_{N1}^R & -\Sigma_{N2}^R & -\Sigma_{N3}^R & \cdots & t_{NN-1} - \Sigma_{NN-1}^R & E - D_N - \Sigma_{NN}^{RB} - \Sigma_{NN}^R \end{pmatrix}^{-1}.$$

In the first part of Lake's paper [4], all the interaction self-energies Σ^R were set equal to 0 and only the boundary self-energies Σ_{11}^{RB} and Σ_{NN}^{RB} introduced in equation (3.6) remain. The size of the matrix is $N \times N$ and the full matrix must be inverted N_E (number of energy points) \times N_k (number of wave vector k points) times. The number of energy points N_E must be quite large because if the resonant levels are sharp, a fine energy discretization is required to take account of them.

The matrix equation can not be solved as long as the contact Green's functions g_{00}^R and g_{N+1N+1}^R are not known because they are included in the boundary self-energies Σ_{11}^{RB} and Σ_{NN}^{RB} . In order to get them, one recalls equation (2.81) from section 2.6 and sets Σ_{LL} equal to 0. One has therefore for the left reservoir

$$\sum_{\gamma=-N_L+1}^0 [(E - D_\alpha) \delta_{\alpha\gamma} + t_{\alpha\gamma}] g_{\gamma\beta}^R = \delta_{\alpha\beta}. \quad (3.9)$$

A similar equation can be found for the right reservoir. Eq. (3.9) can also be written in a matrix form but the first equation presents some difficulties, because it has to account for the coupling with the semi-infinite lead. One has therefore

$$(E - D_{-N_L+1}) g_{-N_L+1, -N_L+1}^R + t_{-N_L+1, -N_L+2} g_{-N_L+2, -N_L+1}^R + \underbrace{t_{-N_L+1, -N_L} g_{-N_L, -N_L+1}^R}_{\Sigma_{-N_L+1, -N_L+1}^{RB} g_{-N_L+1, -N_L+1}^R} = 1, \quad (3.10)$$

where $\Sigma_{-N_L+1, -N_L+1}^{RB} = (-t_{-N_L+1, -N_L}) g_{-N_L, -N_L}^R (-t_{-N_L, -N_L+1})$ represents the coupling with the lead after Eq. (2.82) and $g_{-N_L, -N_L}^R$ is the first Green's function in

the lead when lead and reservoir are not coupled ($t_{-N_L, -N_L+1} = t_{-N_L+1, -N_L} = 0$). It will be evaluated with the following assumptions: the potential for layers $\gamma = [-\infty, \dots, -N_L]$ is equal to the potential at layer $\gamma = -N_L + 1$ (flat band condition), the carriers are in equilibrium (Fermi distribution), there is no interaction, and the Green's functions behave like plane-waves in this region, i.e. $g_{\alpha\beta}^R \propto e^{ik_e|\alpha-\beta|\Delta}$ (this is easily proved by solving the retarded Green's function equation of motion for flat band condition. k_e is the longitudinal wave vector in the emitter contact). This implies that

$$\begin{aligned} g_{-N_L-2, -N_L}^R &= e^{ik_e\Delta} g_{-N_L-1, -N_L}^R \\ g_{-N_L-1, -N_L}^R &= e^{ik_e\Delta} g_{-N_L, -N_L}^R. \end{aligned} \quad (3.11)$$

Inserting these results into Dyson's equation for $g_{-N_L, -N_L}^R$ and $g_{-N_L-1, -N_L}^R$ yields

$$\begin{aligned} (E - D_{-N_L})g_{-N_L, -N_L}^R + t_{-N_L, -N_L+1} \underbrace{g_{-N_L-1, -N_L}^R}_{e^{ik_e\Delta} g_{-N_L, -N_L}^R} \\ + \underbrace{t_{-N_L, -N_L+1}}_0 g_{-N_L+1, -N_L}^R &= 1 \\ (E - D_{-N_L-1})g_{-N_L-1, -N_L}^R + t_{-N_L-1, -N_L} \underbrace{g_{-N_L, -N_L}^R}_{e^{-ik_e\Delta} g_{-N_L-1, -N_L}^R} \\ + t_{-N_L-1, -N_L-2} \underbrace{g_{-N_L-2, -N_L}^R}_{e^{ik_e\Delta} g_{-N_L-1, -N_L}^R} &= 0. \end{aligned} \quad (3.12)$$

Two different conditions are obtained from these equations, if one recalls the flat band behavior of the lead ($D_{-N_L-1} = D_{-N_L}$ and $t_{-N_L, -N_L+1} = t_{-N_L-1, -N_L} = t_{-N_L-1, -N_L-2} = t_e$)

$$\begin{aligned} (E - D_{-N_L} + t_e e^{ik_e\Delta})g_{-N_L, -N_L}^R &= 1 \\ (E - D_{-N_L} + t_e e^{ik_e\Delta} + t_e e^{-ik_e\Delta}) &= 0 \end{aligned} \quad (3.13)$$

where the insertion of the second condition into the first one enables to find a value for the unknown Green's function $g_{-N_L, -N_L}^R$ and thus for the self-energy $\Sigma_{-N_L+1, -N_L+1}^{RB}$ coupling the reservoir with the semi-infinite lead

$$g_{-N_L, -N_L}^R = -\frac{e^{ik_e\Delta}}{t_e} \quad \text{and} \quad \Sigma_{-N_L+1, -N_L+1}^{RB} = -t_e e^{ik_e\Delta}. \quad (3.14)$$

Then one calculates the longitudinal wave vector k_e with the help of the second condition

$$k_e = \frac{1}{\Delta} \arccos\left(\frac{D_{-N_L} - E}{2t_e}\right). \quad (3.15)$$

The calculated retarded self-energy $\Sigma_{-N_L+1, -N_L+1}^{RB}$, the condition for k_e and equation (3.9) are the starting points to construct the matrix equation for the left reservoir, the emitter, (the same procedure holds for the right reservoir, the collector)

$$[g^{Re}] = \begin{pmatrix} E - D_{-N_L+1} - \Sigma_{-N_L+1, -N_L+1}^{RB} & t_{-N_L+1, -N_L+2} & 0 & \cdots & 0 & 0 \\ t_{-N_L+2, -N_L+1} & E - D_{-N_L+2} & t_{-N_L+2, -N_L+3} & \cdots & 0 & 0 \\ 0 & t_{-N_L+3, -N_L+2} & E - D_{-N_L+3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & E - D_{-1} & t_{-1,0} \\ 0 & 0 & 0 & \cdots & t_{0,-1} & E - D_0 \end{pmatrix}^{-1}.$$

True bound states may be present in the spectrum of g_{00}^{Re} (and also g_{N+1N+1}^{Rc}) since the transfer elements t_{01} and t_{10} are set to zero (g^{Re} represent the exact solution of the emitter reservoir when emitter and device are uncoupled). To give a realistic energy width to these states, an energy-dependent optical potential, $i\eta$, is added to the diagonal element of the matrix $(g^{Re})^{-1}$. The originality in the treatment of the boundary conditions comes from the fact that carriers are not directly injected from the reservoirs with varying potential but from the semi-infinite leads. Quantum transport means calculating carrier and current density as described in section 2.7. To achieve this goal, the lesser Green's function $G_{ij}^<$ is required. Thus, one finds with the boundary conditions from section 2.6

$$G_{ij}^< = \sum_{mn \in N} \{ G_{im}^R \Sigma_{mn}^< G_{nj}^A \} + G_{i1}^R \underbrace{(-t_{10})g_{00}^<(-t_{01})}_{\Sigma_{11}^{<B}} G_{1j}^A + G_{iN}^R \underbrace{(-t_{NN+1})g_{N+1N+1}^<(-t_{N+1N})}_{\Sigma_{NN}^{<B}} G_{Nj}^A. \quad (3.16)$$

$g_{00}^<$ and $g_{NN}^<$ can be obtained from the fluctuation-dissipation theorem (section 1.3.3)

$$\begin{aligned} g_{00}^< &= -f^e (g_{00}^{Re} - g_{00}^{Ae}) = if^e A_{00} \\ g_{N+1N+1}^< &= -f^c (g_{N+1N+1}^{Rc} - g_{N+1N+1}^{Ac}) = if^c A_{N+1N+1} \end{aligned} \quad (3.17)$$

and

$$\begin{aligned} \Sigma_{11}^{<B} &= (-t_{10})g_{00}^<(-t_{01}) = if^e(-t_{10})A_{00}(-t_{01}) = if^e \Gamma_{11}^e \\ \Sigma_{11}^{>B} &= (-t_{10})g_{00}^>(-t_{01}) = i(f^e - 1)(-t_{10})A_{00}(-t_{01}) = i(f^e - 1)\Gamma_{11}^e \\ \Sigma_{NN}^{<B} &= (-t_{NN+1})g_{N+1N+1}^<(-t_{N+1N}) = if^c \Gamma_{NN}^c \\ \Sigma_{NN}^{>B} &= (-t_{NN+1})g_{N+1N+1}^>(-t_{N+1N}) = i(f^c - 1)\Gamma_{NN}^c. \end{aligned} \quad (3.18)$$

The four last equations result from (2.104) and are always valid.

All the above considerations form a closed set of equations with the same properties as (2.45). The last open point is the calculation of the self-energies Σ^R and $\Sigma^<$. Some examples are available in section 2.5.3 but general expressions can also be found in

the literature [2, 5, 4, 13, 3].

The final step consists in computing carrier and current density from equations (2.89) and (2.103), respectively. The calculation flow looks as follows

1. To start the simulation, the non-interacting Green's functions $G_0^{R,A}$ and $G_0^{<,>}$ are evaluated from the definition in section 2.5.1. They are then used to calculate the first iterated self-energies $\Sigma^{R,A}$ and $\Sigma^{<,>}$.
2. $G^{R,A}$ is calculated with the matrix equation for $[G^R]$ described in this section and the actual values of the self-energies $\Sigma^{R,A}$ and $\Sigma^{<,>}$. This enables the computation of $G^{<,>}$ with equation (3.16).
3. The updated values of $G^{R,A}$ and $G^{<,>}$ are used to calculate new self-energies $\Sigma^{R,A}$ and $\Sigma^{<,>}$ as described in section 2.5.3, and to calculate the new Hartree potential which goes directly into the Hamiltonian H_0 through $V(z)$. This is equivalent to compute Poisson's equation with the carrier density given in equation (2.89) and to modify the device potential. If the self-consistent iteration procedure between the Green's functions and the self-energies has converged, one can proceed to the next step, otherwise, the loop between step 2 and step 3 must be repeated until convergence is achieved.
4. The self-consistent Green's functions and self-energies obtained from the definitive device potential are used to calculate the current density with equation (2.103).

3.1.1.1 Ballistic Transport

An interesting method is presented in the paper of Lake to solve the matrix equation for $[G^R]$, but it works only for ballistic transport, where all the self-energies disappear except the boundary terms. With this method, one calculates only the Green's functions required for the carrier and current density in equations (2.89) and (2.107), respectively

$$\begin{aligned}
n(z_n) &= \frac{1}{\Delta} \int_{z_n - \frac{\Delta}{2}}^{z_n + \frac{\Delta}{2}} dz n(z) = -\frac{i}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} G_{nn}^<(\mathbf{k}_t; E) \\
&= -\frac{i}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \{ [G_{n1}^R \Sigma_{11}^{<B} G_{1n}^A](\mathbf{k}_t; E) + [G_{nN}^R \Sigma_{NN}^{<B} G_{Nn}^A](\mathbf{k}_t; E) \} \\
&= \frac{1}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \{ f^e [G_{n1}^R \Gamma_{11}^e G_{1n}^A](\mathbf{k}_t; E) + f^c [G_{nN}^R \Gamma_{NN}^c G_{Nn}^A](\mathbf{k}_t; E) \} \\
&= \frac{1}{A\Delta} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} \{ (f^e - f^c) [G_{n1}^R \Gamma_{11}^e G_{1n}^A](\mathbf{k}_t; E) + f^c A_{nn}(\mathbf{k}_t; E) \} \\
J &= \frac{e}{\hbar A} \sum_{\mathbf{k}_t, \sigma} \int \frac{dE}{2\pi} [\Gamma_{11}^e G_{1N}^R \Gamma_{NN}^c G_{N1}^A](\mathbf{k}_t; E) (f^e(E) - f^c(E))
\end{aligned}$$

$$= \frac{e}{\hbar A} \sum_{\mathbf{k}\mathbf{t}, \sigma} \int \frac{dE}{2\pi} [\Gamma_{11}^e (A_{11} - G_{11}^R \Gamma_{11}^e G_{11}^A)] (\mathbf{k}\mathbf{t}; E) (f^e(E) - f^c(E)) \quad (3.19)$$

because only Γ_{11}^e and Γ_{NN}^c are different from 0 and

$$\begin{aligned} A_{nn} &= i(G_{nn}^R - G_{nn}^A) = i(G_{nn}^> - G_{nn}^<) \\ &= i([G_{n1}^R \Sigma_{11}^{>B} G_{1n}^A - G_{n1}^R \Sigma_{11}^{<B} G_{1n}^A] + [G_{nN}^R \Sigma_{NN}^{>B} G_{Nn}^A - G_{nN}^R \Sigma_{NN}^{<B} G_{Nn}^A]) \\ &= G_{n1}^R \Gamma_{11}^e G_{1n}^A + G_{nN}^R \Gamma_{NN}^c G_{Nn}^A \end{aligned} \quad (3.20)$$

For ballistic transport, the first column and the diagonal of the matrix representing G^R are needed. A recursive algorithm providing them is developed. In the following derivation, all upper case G 's and lower case g 's are retarded Green's functions and hence one will drop the superscript R . Upper case G 's are reserved for the exact Green's function elements, the term g^r indicates that the Green's function takes into account everything on the right exactly with the coupling elements immediately to the left set to 0. For instance, to compute g_{nn}^r , t_{nn-1} and t_{n-1n} are equal to 0. The equation for $g_{n:N,n:N}^r$ and $g_{n+1:N,n+1:N}^r$ can be written as

$$T_{n:N,n:N} g_{n:N,n:N}^r = \mathbf{1} \quad T_{n+1:N,n+1:N} g_{n+1:N,n+1:N}^r = \mathbf{1}, \quad (3.21)$$

where T is a tri-diagonal matrix equivalent to the one resulting from equation (3.8) but with all the self-energies equal to 0 except the Σ^{RB} 's. In matrix form, one has

$$\begin{pmatrix} T_{nn} & T_{n,n+1:N} \\ T_{n+1:N,n} & T_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} g_{nn}^r & g_{n,n+1:N}^r \\ g_{n+1:N,n}^r & g_{n+1:N,n+1:N}^r \end{pmatrix} = \begin{pmatrix} 1 & \mathbf{0}_{n,n+1:N} \\ \mathbf{0}_{n+1:N,n} & \mathbf{1}_{n+1:N,n+1:N} \end{pmatrix}$$

with $T_{n,n+1:N} = [T_{nn+1} \ 0 \ \cdots \ 0]$ and $T_{n+1:N,n} = [T_{n+1n} \ 0 \ \cdots \ 0]^\dagger$. One can extract two equations

$$\begin{aligned} T_{nn} g_{nn}^r + T_{n,n+1:N} g_{n+1:N,n}^r &= 1 \\ T_{n+1:N,n} g_{nn}^r + T_{n+1:N,n+1:N} g_{n+1:N,n}^r &= \mathbf{0}_{n+1:N,n}. \end{aligned} \quad (3.22)$$

From the first one and the properties of T described above,

$$T_{nn} g_{nn}^r + T_{nn+1} g_{n+1n}^r = 1, \quad (3.23)$$

and from the second equation

$$\begin{aligned} (g_{n+1:N,n+1:N}^r)^{-1} g_{n+1:N,n}^r &= -T_{n+1:N,n} g_{nn}^r \\ g_{n+1:N,n}^r &= -g_{n+1:N,n+1:N}^r T_{n+1:N,n} g_{nn}^r \\ g_{n+1,n}^r &= -g_{n+1n+1}^r T_{n+1n} g_{nn}^r \end{aligned} \quad (3.24)$$

The combination of both results yields

$$\boxed{g_{nn}^r = (T_{nn} - T_{nn+1} g_{n+1n+1}^r T_{n+1n})^{-1}}. \quad (3.25)$$

Once $g_{N+N_R, N+N_R}$ (which is done with the boundary and flat band conditions described in equation (3.11)) is known, all the other g^r 's can be found. For the exact Green's functions, the equation to be solved is

$$\begin{pmatrix} T_{1:n,1:n} & T_{1:n,n+1:N} \\ T_{n+1:N,1:n} & T_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} G_{1:n,1:n} & G_{1:n,n+1:N} \\ G_{n+1:N,1:n} & G_{n+1:N,n+1:N} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{1:n,1:n} & \mathbf{0}_{1:n,n+1:N} \\ \mathbf{0}_{n+1:N,1:n} & \mathbf{1}_{n+1:N,n+1:N} \end{pmatrix}$$

or

$$\begin{pmatrix} G_{1:n,1:n} & G_{1:n,n+1:N} \\ G_{n+1:N,1:n} & G_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} T_{1:n,1:n} & T_{1:n,n+1:N} \\ T_{n+1:N,1:n} & T_{n+1:N,n+1:N} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{1:n,1:n} & \mathbf{0}_{1:n,n+1:N} \\ \mathbf{0}_{n+1:N,1:n} & \mathbf{1}_{n+1:N,n+1:N} \end{pmatrix}.$$

Two different equations are extracted from these systems, coupling $G_{1:n,1:n}$ and $G_{n+1:N,n+1:N}$

$$\begin{aligned} T_{n+1:N,1:n}G_{1:n,n+1:N} + T_{n+1:N,n+1:N}G_{n+1:N,n+1:N} &= \mathbf{1}_{n+1:N,n+1:N} \\ G_{1:n,1:n}T_{1:n,n+1:N} + G_{1:n,n+1:N}T_{n+1:N,n+1:N} &= \mathbf{0}_{1:n,n+1:N}. \end{aligned} \quad (3.26)$$

From the first line of (3.26) and with consideration of (3.21), one obtains

$$G_{n+1:N,n+1:N} = g_{n+1:N,n+1:N}^r + g_{n+1:N,n+1:N}^r T_{n+1:N,1:n} G_{1:n,n+1:N}, \quad (3.27)$$

from the second

$$G_{1:n,n+1:N} = -G_{1:n,1:n}T_{1:n,n+1:N}g_{n+1:N,n+1:N}^r \quad (3.28)$$

and the combination of both delivers

$$\begin{aligned} G_{n+1:N,n+1:N} &= g_{n+1:N,n+1:N}^r \\ &- g_{n+1:N,n+1:N}^r T_{n+1:N,1:n} G_{1:n,1:n} T_{1:n,n+1:N} g_{n+1:N,n+1:N}^r. \end{aligned} \quad (3.29)$$

Because of the properties of the tri-diagonal matrix T , one element of the last equation can be isolated

$$\boxed{G_{n+1n+1} = g_{n+1n+1}^r + g_{n+1,n+1}^r T_{n+1n} G_{nn} T_{nn+1} g_{n+1n+1}^r.} \quad (3.30)$$

It remains to determine the first point $G(1, 1)$ to be able to reconstruct all the other diagonal Green's functions recursively. It obeys the following equation

$$(E - D_1)G_{1,1} + t_{12}G_{21} - \Sigma_{11}^{RB}G_{11} = 1. \quad (3.31)$$

From the first matrix equation above, one has

$$T_{n+1:N,1:n}G_{1:n,1:n} + T_{n+1:N,n+1:N}G_{n+1:N,1:n} = \mathbf{0}_{n+1:N,1:n} \quad (3.32)$$

which can be written as

$$G_{n+1:N,1:n} = -g_{n+1:N,n+1:N}^r T_{n+1:N,1:n} G_{1:n,1:n}. \quad (3.33)$$

The isolation of the first element yields

$$\boxed{G_{n+11} = -g_{n+1n+1}^r T_{n+1n} G_{n1}} \quad (3.34)$$

and for the case $n = 1$, one finds $G_{21} = -g_{22}^r T_{21} G_{11}$, one puts this result into equation (3.31), and one obtains

$$\boxed{G_{1,1} = (E - D_1 - t_{12} g_{22}^r t_{21} - \Sigma_{11}^{RB})^{-1}}. \quad (3.35)$$

With equations (3.30) and (3.34), all the elements required to compute carrier and current density in the ballistic regime are determined recursively in an efficient way. If one now includes self-energies, the algorithm does not work anymore for two reasons

- the properties of the matrix T disappear because T is no more a tri-diagonal matrix but is full,
- even if one can find an algorithm to isolate the Green's functions required for carrier and current density, the self-energies needed for that are calculated with the full set of Green's functions.

Furthermore, one also needs the lesser Green's functions $G_{nn}^<$ for all the points in order to calculate the new self-consistent potential resulting from the charge density. They can be obtained from the advanced and retarded Green's functions or calculated with a recursive algorithm: as for the retarded case, upper case G 's are reserved for the exact Green's functions while the terms g^n indicates that the Green's functions take into account every point greater or equal to n exactly with the coupling $T_{nn-1} = 0$. The equations for $g_{n:N,n:N}^<n$ and $g_{n+1:N,n+1:N}^{<n+1}$ are therefore

$$\begin{aligned} T_{n:N,n:N} g_{n:N,n:N}^<n &= \Sigma_{n:N,n:N}^< g_{n:N,n:N}^{An} \\ T_{n+1:N,n+1:N} g_{n+1:N,n+1:N}^{<n+1} &= \Sigma_{n+1:N,n+1:N}^< g_{n+1:N,n+1:N}^{An+1}. \end{aligned} \quad (3.36)$$

$\Sigma_{n:N,n:N}^<$ and $\Sigma_{n+1:N,n+1:N}^<$ are diagonal matrices representing the boundary conditions of the lesser Green's functions. In case of Büttiker probes used as scattering centers, they also represent the diagonal scattering self-energies. In matrix form, equation (3.36) can be written as

$$\begin{pmatrix} T_{nn} & T_{n,n+1:N} \\ T_{n+1:N,n} & T_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} g_{nn}^<n & g_{n,n+1:N}^<n \\ g_{n+1:N,n}^<n & g_{n+1:N,n+1:N}^<n \end{pmatrix} = \begin{pmatrix} \Sigma_{nn}^< & \mathbf{0}_{n,n+1:N} \\ \mathbf{0}_{n+1:N,n} & \Sigma_{n+1:N,n+1:N}^< \end{pmatrix} \cdot \begin{pmatrix} g_{nn}^{An} & g_{n,n+1:N}^{An} \\ g_{n+1:N,n}^{An} & g_{n+1:N,n+1:N}^{An} \end{pmatrix}. \quad (3.37)$$

Two coupled equations can be extracted from (3.37)

$$\begin{cases} T_{nn} g_{nn}^<n + T_{n,n+1:N} g_{n+1:N,n}^<n &= \Sigma_{nn}^< g_{nn}^{An} \\ T_{n+1:N,n} g_{nn}^<n + T_{n+1:N,n+1:N} g_{n+1:N,n}^<n &= \Sigma_{n+1:N,n+1:N}^< g_{n+1:N,n}^{An} \end{cases} \quad (3.38)$$

The second equation can be transformed, with the help of the property coming from the lower case retarded Green's functions $T_{n+1:N,n+1:N} = (g_{n+1:N,n+1:N}^{Rn+1})^{-1}$, into

$$g_{n+1:N,n}^<n = - \underbrace{g_{n+1:N,n+1:N}^{Rn+1} T_{n+1:N,n} g_{nn}^<n}_{(1)} + \underbrace{g_{n+1:N,n+1:N}^{Rn+1} \Sigma_{n+1:N,n+1:N}^< g_{n+1:N,n}^{An}}_{(2)}. \quad (3.39)$$

Furthermore, the lower case advanced Green's function $g_{n+1:N,n}^{An}$ is given by equation (3.24)

$$g_{n+1:N,n}^{An} = -g_{n+1:N,n+1:N}^{An+1} T_{n+1:N,n}^* g_{nn}^{An}. \quad (3.40)$$

The first part of equation (3.39) becomes

$$\begin{aligned} (1) & : g_{n+1:N,n+1:N}^{Rn+1} T_{n+1:N,n} g_{nn}^{<n} \\ & : g_{n+1:N,n+1}^{Rn+1} T_{n+1,n} g_{nn}^{<n} \end{aligned} \quad (3.41)$$

Then inserting result (3.40) into the second part of equation (3.39) yields the following expression

$$\begin{aligned} (2) & : g_{n+1:N,n+1:N}^{Rn+1} \Sigma_{n+1:N,n+1:N} g_{n+1:N,n}^{An} \\ & \quad - \underbrace{g_{n+1:N,n+1:N}^{An+1} T_{n+1:N,n}^* g_{nn}^{An}}_{- T_{n+1:N,n+1:N} g_{n+1:N,n+1:N}^{<n+1}} \\ & \quad - \underbrace{T_{n+1:N,n+1:N} g_{n+1:N,n+1:N}^{<n+1}}_{- \mathbf{I}_{n+1:N,n+1:N}} \\ & : -g_{n+1:N,n+1:N}^{<n+1} T_{n+1:N,n}^* g_{nn}^{An}. \end{aligned} \quad (3.42)$$

This gives for $g_{n+1:N,n}^{<n}$ and for its reduced form $g_{n+1,n}^{<n}$

$$\begin{aligned} g_{n+1:N,n}^{<n} & = -g_{n+1:N,n+1}^{Rn+1} T_{n+1,n} g_{nn}^{<n} - g_{n+1:N,n+1}^{<n+1} T_{n+1,n}^* g_{nn}^{An} \\ g_{n+1,n}^{<n} & = -g_{n+1,n+1}^{Rn+1} T_{n+1,n} g_{nn}^{<n} - g_{n+1,n+1}^{<n+1} T_{n+1,n}^* g_{nn}^{An}. \end{aligned} \quad (3.43)$$

$g_{n+1:N,n}^{<n}$ is then inserted into the first equation of (3.60) to obtain a recursive for $g_{nn}^{<n}$ depending on $g_{n+1,n+1}^{<n+1}$

$$\underbrace{\left(T_{nn} - T_{n,n+1} g_{n+1,n+1}^{Rn+1} T_{n+1,n} \right)}_{\left(g_{nn}^{Rn} \right)^{-1}} g_{nn}^{<n} = T_{n,n+1} g_{n+1,n+1}^{<n+1} T_{n+1,n}^* g_{nn}^{An} + \Sigma_{nn} g_{nn}^{An} \quad (3.44)$$

which yields

$$\boxed{g_{nn}^{<n} = g_{nn}^{Rn} T_{n,n+1} g_{n+1,n+1}^{<n+1} T_{n+1,n}^* g_{nn}^{An} + g_{nn}^{Rn} \Sigma_{nn} g_{nn}^{An}} \quad (3.45)$$

Starting from $g_{N+N_R,N+N_R}^{<N+N_R}$ and going back to $g_{-N_L,-N_L}^{<-N_L}$, all the lower case Green's functions can be obtained. For the exact Green's functions, the equation to be solved is

$$\begin{pmatrix} T_{1:n1:n} & T_{1:n,n+1:N} \\ T_{n+1:N,1:n} & T_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} G_{1:n1:n}^{<} & G_{1:n,n+1:N}^{<} \\ G_{n+1:N,1:n}^{<} & G_{n+1:N,n+1:N}^{<} \end{pmatrix} = \begin{pmatrix} \Sigma_{1:n1:n}^{<} & \mathbf{0}_{1:n,n+1:N} \\ \mathbf{0}_{n+1:N,1:n} & \Sigma_{n+1:N,n+1:N} \end{pmatrix} \cdot \begin{pmatrix} G_{1:n1:n}^A & G_{1:n,n+1:N}^A \\ G_{n+1:N,1:n}^A & G_{n+1:N,n+1:N}^A \end{pmatrix} \quad (3.46)$$

or

$$\begin{pmatrix} G_{1:n1:n}^{<} & G_{1:n,n+1:N}^{<} \\ G_{n+1:N,1:n}^{<} & G_{n+1:N,n+1:N}^{<} \end{pmatrix} \cdot \begin{pmatrix} T_{1:n1:n}^* & T_{1:n,n+1:N}^* \\ T_{n+1:N,1:n}^* & T_{n+1:N,n+1:N}^* \end{pmatrix} = \\ \begin{pmatrix} G_{1:n1:n}^R & G_{1:n,n+1:N}^R \\ G_{n+1:N,1:n}^R & G_{n+1:N,n+1:N}^R \end{pmatrix} \cdot \begin{pmatrix} \Sigma_{1:n1:n}^{<} & \mathbf{0}_{1:n,n+1:N} \\ \mathbf{0}_{n+1:N,1:n} & \Sigma_{n+1:N,n+1:N}^{<} \end{pmatrix}. \quad (3.47)$$

Two different equations are extracted from these systems, one coupling $G_{n+1:N,n+1:N}^{<}$ (which is searched) to $G_{1:n,n+1:N}^{<}$, and the other $G_{1:n,n+1:N}^{<}$ to $G_{1:n,1:n}^{<}$ (which is known) in order to obtain a recursive algorithm between $G_{n+1:N,n+1:N}^{<}$ and $G_{1:n,1:n}^{<}$. For that purpose, one uses

$$\begin{cases} T_{n+1:N,1:n} G_{1:n,n+1:N}^{<} + T_{n+1:N,n+1:N} G_{n+1:N,n+1:N}^{<} = \Sigma_{n+1:N,n+1:N}^{<} G_{n+1:N,n+1:N}^A, \\ G_{1:n,1:n}^{<} T_{1:n,n+1:N}^* + G_{1:n,n+1:N}^{<} T_{n+1:N,n+1:N}^* = G_{1:n,n+1:N}^R \Sigma_{n+1:N,n+1:N}^{<}. \end{cases} \quad (3.48)$$

One starts with the first equation of (3.48) and separates the result into two parts

$$G_{n+1:N,n+1:N}^{<} = \underbrace{-g_{n+1:N,n+1:N}^{Rn+1} T_{n+1:N,1:n} G_{1:n,n+1:N}^{<}}_{(1)} + \underbrace{g_{n+1:N,n+1:N}^{Rn+1} \Sigma_{n+1:N,n+1:N}^{<} G_{n+1:N,n+1:N}^A}_{(2)}. \quad (3.49)$$

The first part (1) of equation (3.49) can not be simplified for the moment. However, some work can be accomplished for the second one (2)

$$(2) : g_{n+1:N,n+1:N}^{Rn+1} \Sigma_{n+1:N,n+1:N}^{<} G_{n+1:N,n+1:N}^A \\ \underbrace{g_{n+1:N,n+1:N}^{An+1} \left(1 + T_{n+1:N,1:n}^* G_{1:n,1:n}^A T_{1:n,n+1:N}^* g_{n+1:N,n+1:N}^{An+1} \right)}_{T_{n+1:N,n+1:N} g_{n+1:N,n+1:N}^{<n+1}} \\ \mathbf{I}_{n+1:N,n+1:N}.$$

The second equation from the system developed in (3.48) is also composed of two parts

$$G_{1:n,n+1:N}^{<} = \underbrace{-G_{1:n,1:n}^{<} T_{1:n,n+1:N}^* g_{n+1:N,n+1:N}^{An+1}}_{(3)} + \underbrace{G_{1:n,n+1:N}^R \Sigma_{n+1:N,n+1:N}^{<} g_{n+1:N,n+1:N}^{An+1}}_{(4)}. \quad (3.50)$$

For part (4), the two last terms are replaced according to equation (3.36) while the first part is expanded with the help of (3.28). As consequence, one obtains

$$(4) : -G_{1:n,1:n}^R T_{1:n,n+1:N} g_{n+1:N,n+1:N}^{<n+1}. \quad (3.51)$$

It remains to evaluate the sum of (3) and (4)

$$G_{1:n,n+1:N}^{<} = -G_{1:n,n}^{<} T_{n,n+1}^* g_{n+1,n+1:N}^{An+1} - G_{1:n,n}^R T_{n,n+1} g_{n+1,n+1:N}^{<n+1} \quad (3.52)$$

to insert it into part (1), which is added to part (2) to find the desired $G_{n+1:N,n+1:N}^{<}$

$$\begin{aligned} G_{n+1:N,n+1:N}^{<} &= g_{n+1:N,n+1:N}^{<n+1} + g_{n+1:N,n+1}^{<n+1} T_{n+1,n}^* G_{n,n}^A T_{n,n+1}^* g_{n+1,n+1:N}^{An+1} + \\ &\quad g_{n+1:N,n+1}^{Rn+1} T_{n+1,n} G_{n,n}^{<} T_{n,n+1}^* g_{n+1,n+1:N}^{An+1} + \\ &\quad g_{n+1:N,n+1}^{Rn+1} T_{n+1,n} G_{n,n}^R T_{n,n+1} g_{n+1,n+1:N}^{<n+1} \end{aligned} \quad (3.53)$$

or

$$\boxed{G_{n+1,n+1}^{<} = g_{n+1,n+1}^{<n+1} + g_{n+1,n+1}^{<n+1} T_{n+1,n}^* G_{n,n}^A T_{n,n+1}^* g_{n+1,n+1}^{An+1} + g_{n+1,n+1}^{Rn+1} T_{n+1,n} G_{n,n}^{<} T_{n,n+1}^* g_{n+1,n+1}^{An+1} + g_{n+1,n+1}^{Rn+1} T_{n+1,n} G_{n,n}^R T_{n,n+1} g_{n+1,n+1}^{<n+1}} \quad (3.54)$$

This concludes the derivation of the recursive algorithm for the lesser Green's function. It can be applied in the leads for example, or in the presence of Büttiker probes as scattering centers.

3.1.1.2 Multiple Sequential Scattering

The last part of Lake's paper [4] is dedicated to the solution of the quantum transport problem in resonant tunneling devices when scattering processes are included but where a truncation is applied in the self-consistent calculation of the Green's functions and the self-energies. The algorithm is well explained in the paper, containing a lot of pictures describing the procedure and the possible simplifications. The only inelastic scattering mechanism which is included in the algorithm, is the carrier-optical-phonon interaction. However, for convenience, the principle integral present in equation (2.65) is neglected.

3.1.2 Strength and Weakness

The model presented in [4] contains all the desirable effects like carrier-phonon interactions, impurity scattering or quantum mechanical calculation of the charge and the current except the carrier-carrier interactions which are responsible for Coulomb blockade in very small devices.

A very efficient algorithm is derived to take into account large reservoirs in the calculation of the Green's functions through boundary self-energies. This allows one to concentrate on the device physics but without neglecting the injection regions, where the potential does not need to be flat.

The paper of Lake [4] also presents an original method to compute the Green's functions for ballistic transport (i.e., when all the interactions are neglected) where the diagonal and left column elements of the matrix Green's functions are found recursively. The only disadvantage of this method is that it does not work if self-energies are present so that it restricts its domain of use.

3.2 Two-dimensional Nanotransistors

The diagram illustrates a 2D grid representing a semiconductor device structure. The grid is bounded by semi-infinite boundaries on the left and right. The vertical axis is labeled 'y' and the horizontal axis is labeled 'x'. The grid is divided into regions: 'S' (Source) on the left, 'P' (P-type) in the center, and 'D' (Drain) on the right. The grid is labeled with coordinates: $-L_y/2$, $-L_x/2$, $L_x/2$, $L_y/2$. The grid is also labeled with indices: -1 , 0 , 1 , q , $q+1$, N_y+1 , N_y+2 , N_y+3 . The grid is labeled with 'oxide' and 'semi-infinite boundary'.

Figure 3.2: Nanoscale MOSFET with 2D Grid. Each column q corresponds to a submatrix of equation (3.40).

3.2.1 Model Summary

The model presented in [14] is a 2D generalization of Lake's one explained in the last section, but it is derived only for ballistic transport. Therefore, it is not necessary to present all the equations, but just their 2D form. It will be assumed, as in figure 3.2, that the transistor is situated in the $x-y$ plane and that the carriers can move freely in the z direction. The eigenfunction expansion of the Green's functions with orbital functions (or pseudo-Wannier functions) will contain four indices, two for x (ii') and two for y (jj'), and it will depend on k_z : $G_{ii'jj'}(k_z; t_1 t_1')$,

$$\begin{aligned} G(11') &= \frac{1}{L_z} \sum_{ii'} \sum_{jj'} \sum_{k_z} \phi_{ij}(xy) G_{ii'jj'}(k_z; tt') \phi_{i'j'}^*(x'y') e^{ik_z(z-z')}, \\ G_{ii'jj'}(k_z; tt') &= \int d\mathbf{r} \int d\mathbf{r}' \phi_{ij}^*(xy) G(11') \phi_{i'j'}(x'y') e^{-ik_z(z-z')}, \end{aligned} \quad (3.55)$$

where $\phi_{ij}(xy)$ is an orbital or pseudo-Wannier function situated at position (x_i, y_j) . In the stationary regime, the Green's functions depend only on the difference $t - t'$, thus they can be Fourier transformed and depend only on the energy E .

The equations of motion for the retarded (G^R) and the lesser ($G^<$) Green's functions are then derived from (2.45)

$$\begin{aligned} EG_{ii'jj'}^<(k_z; E) - \sum_{i_1 j_1} h_{ii_1 jj_1} G_{i_1 i' j_1 j'}^<(k_z; E) &= \sum_{i_1 j_1} \Sigma_{ii_1 jj_1}^R(k_z; E) G_{i_1 i' j_1 j'}^<(k_z; E) + \\ &\quad \sum_{i_1 j_1} \Sigma_{ii_1 jj_1}^<(k_z; E) G_{i_1 i' j_1 j'}^A(k_z; E) \\ EG_{ii'jj'}^R(k_z; E) - \sum_{i_1 j_1} h_{ii_1 jj_1} G_{i_1 i' j_1 j'}^R(k_z; E) &= \delta_{ii'} \delta_{jj'} + \sum_{i_1 j_1} \Sigma_{ii_1 jj_1}^R(k_z; E) G_{i_1 i' j_1 j'}^R(k_z; E) \end{aligned} \quad (3.56)$$

where for ballistic transport the self-energies are neglected. The Hamiltonian H_0 is defined by

$$H_0 = -\frac{\hbar^2}{2m^{*x}} \frac{d^2}{dx^2} - \frac{\hbar^2}{2m^{*y}} \frac{d^2}{dy^2} + \frac{\hbar^2 k_z^2}{2m^{*z}} + V(xy) \quad (3.57)$$

and one introduces the transfer matrix $t_{jj'}^{ii'}$ whose elements are (here one will only consider the case with equidistant mesh points, the other case is straightforward and is treated in [14])

$$t_{jj'}^{ii'} = \begin{cases} t_{jj}^{ii\pm 1} = \frac{\hbar^2}{(m_i^{*x} + m_{i\pm 1}^{*x}) \Delta_x^2} & i' = i \pm 1, j' = j, \\ t_{jj\pm 1}^{ii} = \frac{\hbar^2}{(m_j^{*y} + m_{j\pm 1}^{*y}) \Delta_y^2} & i' = i, j' = j \pm 1, \\ 0 & \text{otherwise} \end{cases} \quad (3.58)$$

with $\Delta_x = x_i - x_{i-1}$ and $\Delta_y = y_j - y_{j-1}$, so that the matrix element $h_{ii'jj'}$ are given by

$$h_{ii'jj'} = \int dx \int dy \phi_{ij}^*(xy) H_0 \phi_{i'j'}(xy) \quad (3.59)$$

$$= \begin{cases} h_{iijj} = t_{jj}^{ii+1} + t_{jj}^{ii-1} + t_{jj+1}^{ii} + t_{jj-1}^{ii} + V_{ij} + \frac{\hbar^2 k_z^2}{2m^*z} & i' = i, j' = j \\ h_{ii\pm 1jj} = -t_{jj}^{ii\pm 1} & i' = i \pm 1, j' = j \\ h_{iijj\pm 1} = -t_{jj\pm 1}^{ii} & i' = i, j' = j \pm 1. \\ 0 & \text{otherwise} \end{cases}$$

For the structure defined in figure 3.2, there are N_x points in the x direction running from 1 to N_x and N_y points in the y direction running from 1 to N_y . However it remains to derive the boundary conditions with the help of the procedure developed in section 2.6 to take into account the semi-infinite injection regions. If i and i' are two points between 1 and N_x while j and j' are situated between 1 and N_y , one obtains

$$G_{ii'jj'}^R = g_{ii'jj'}^R + \sum_{i_1 i_2} g_{ii_1 j_1}^R \underbrace{\left(-t_{10}^{i_1 i_1} \right) g_{i_1 i_2 00}^R \left(-t_{01}^{i_2 i_2} \right)}_{\Sigma_{i_1 i_2 11}^{RS}} G_{i_2 i' 1 j'}^R$$

$$+ \sum_{i_1 i_2} g_{ii_1 j_{N_y}}^R \underbrace{\left(-t_{N_y N_y + 1}^{i_1 i_1} \right) g_{i_1 i_2 N_y + 1 N_y + 1}^R \left(-t_{N_y + 1 N_y}^{i_2 i_2} \right)}_{\Sigma_{i_1 i_2 N_y N_y}^{RD}} G_{i_2 i' N_y j'}^R$$

$$+ \sum_{j_1 j_2} g_{i 1 j j_1}^R \underbrace{\left(-t_{j_1 j_1}^{10} \right) g_{00 j_1 j_2}^R \left(-t_{j_2 j_2}^{01} \right)}_{\Sigma_{11 j_1 j_2}^{RG}} G_{1 i' j_2 j'}^R. \quad (3.60)$$

The G 's are exact Green's functions while the g 's are Green's functions when Gate, Drain, Source, and device are not coupled, Σ^{RS} is the boundary self-energy for the source contact, Σ^{RD} for the Drain, and Σ^{RG} for the Gate. Furthermore, $g_{ii'jj'}^R$ obeys the following equation, similar to (3.7), but for ballistic transport

$$\sum_{i_0 \in N_x} \sum_{j_0 \in N_y} \underbrace{\left[(E - h_{ii_0 j j_0}) \delta_{ii_0} \delta_{j j_0} + t_{j j_0}^{ii_0} \right]}_{[g_{ii_0 j j_0}^R]^{-1}} g_{i_0 i' j_0 j'}^R = \delta_{ii'} \delta_{j j'}. \quad (3.61)$$

Operating with $[g_{ii_0 j j_0}^R]^{-1}$ on $G_{i_0 i' j_0 j'}^R$ from equation (3.60) and summing over i_0 and j_0 yields

$$\sum_{i_0 \in N_x} \sum_{j_0 \in N_y} \left[(E - h_{ii_0 j j_0}) \delta_{ii_0} \delta_{j j_0} + t_{j j_0}^{ii_0} \right] G_{i_0 i' j_0 j'}^R = \delta_{ii'} \delta_{j j'} + \delta_{j1} \sum_{i_2} \Sigma_{ii_2 11}^{RS} G_{i_2 i' 1 j'}^R$$

$$+ \delta_{j N_y} \sum_{i_2} \Sigma_{ii_2 N_y N_y}^{RD} G_{i_2 i' N_y j'}^R$$

$$+\delta_{i1} \sum_{j_2} \Sigma_{11j_2}^{RG} G_{1i'j_2j'}^R.$$

This equation can be rewritten as a matrix equation whose size is $(N_x N_y) \times (N_x N_y)$, but made of $N_y \times N_y$ submatrices of size $N_x \times N_x$

$$A \cdot G^R = \mathbf{1}. \quad (3.62)$$

The elements of the matrix A are $A_{jj'}(ii')$, where j, j' indicate in which submatrix the element is and i, i' the place within the submatrix. As consequence, a submatrix $A_{jj'}$ corresponds to a column with a constant y and x running from 1 to N_x in Figure 3.2. In addition to these considerations, if the boundary self-energies $\Sigma_{11j_2}^{RG}$ are set to zero when $j_2 \notin \{j, j \pm 1\}$, then the matrix A is a tri-block-diagonal matrix, allowing the derivation of an efficient algorithm to compute only the required Green's functions determining carrier and current density. This recursive algorithm is similar to Lake's one presented in the previous section and will not be repeated here. In this case, the elements of the matrix A are

$$A_{jj'}^{ii'} = \begin{cases} E - h_{iijj} - \Sigma_{ii11}^{RS} \delta_{j1} - \Sigma_{iiN_y N_y}^{RD} \delta_{jN_y} - \Sigma_{11jj}^{RG} \delta_{i1} & i' = i, j' = j \\ t_{jj}^{ii'} - \Sigma_{ii'11}^{RS} \delta_{j1} - \Sigma_{ii'N_y N_y}^{RD} \delta_{jN_y} & i' \neq i, j' = j \\ t_{jj'}^{ii} - \Sigma_{11jj'}^{RG} \delta_{i1} & i' = i, j' = j \pm 1 \\ 0 & \text{otherwise.} \end{cases} \quad (3.63)$$

To evaluate the boundary Green's functions Σ^{RS} , Σ^{RD} , and Σ^{RG} as they appear in equation (3.60), the lower case Green's functions g^R are required and one obtains them with the same procedure as for the 1D resonant tunneling device: the Green's functions in the separated reservoirs are calculated, using the flat band condition and wave behavior of the Green's functions at the end of the reservoirs.

3.2.1.1 Carrier and Current Density

The quantum transport problem requires the solution of carrier and current density. Thus an equation must be found for them, starting with the carrier density, derived from equation (2.89)

$$\boxed{n(x_i y_j) = -\frac{i}{L_z \Delta_x \Delta_y} \sum_{k_z, \sigma} \int \frac{dE}{2\pi} G_{iijj}^{<}(k_z; E).} \quad (3.64)$$

The continuity equation introduced in (2.92) gives

$$\begin{aligned} \frac{d}{dt} \rho_{ij}(t) &= \lim_{t' \rightarrow t} (-i\hbar) \frac{e}{L_z \Delta_x \Delta_y} \sum_{k_z, \sigma} \left(\frac{d}{dt} G_{iijj}^{<}(k_z; tt') + \frac{d}{dt'} G_{iijj}^{<}(k_z; tt') \right) \\ &= -\frac{J_{ij}(t) - J_{i-1j}(t)}{\Delta_x} - \frac{J_{ij}(t) - J_{ij-1}(t)}{\Delta_y}. \end{aligned} \quad (3.65)$$

For ballistic transport, the evaluation of equation (3.65) yields

$$\frac{d}{dt}\rho_{ij}(t) = -\frac{e}{L_z\Delta_x\Delta_y} \sum_{k_z,\sigma} \sum_{i_1j_1} \left(h_{ii_1jj_1} G_{i_1ij_1j}^<(k_z; tt) - G_{ii_1jj_1}^<(k_z; tt) h_{i_1ij_1j} \right) \quad (3.66)$$

and because $h_{ii_1jj_1}$ is either diagonal in the x (ii_1) or y (jj_1) direction

$$\begin{aligned} \frac{d}{dt}\rho_{ij}(t) = & -\frac{e}{L_z\Delta_x\Delta_y} \sum_{k_z,\sigma} \left\{ \sum_{i_1} \left(h_{ii_1jj} G_{i_1ijj}^<(k_z; tt) - G_{ii_1jj}^<(k_z; tt) h_{i_1ijj} \right) \right. \\ & \left. + \sum_{j_1} \left(h_{iijj_1} G_{iij_1j}^<(k_z; tt) - G_{iij_1j}^<(k_z; tt) h_{iij_1j} \right) \right\} \quad (3.67) \end{aligned}$$

With the ansatz proposed by Caroli in [6], the total current becomes

$$J_{ij} = -\frac{e}{\hbar L_z} \left(\sum_{i_1 \geq i+1} \sum_{i_2 \leq i} \sum_{k_z,\sigma} \int \frac{dE}{2\pi\Delta_y} \left(h_{i_1i_2jj} G_{i_2i_1jj}^<(k_z; E) - G_{i_1i_2jj}^<(k_z; E) h_{i_2i_1jj} \right) \right. \\ \left. \sum_{j_1 \geq j+1} \sum_{j_2 \leq j} \sum_{k_z,\sigma} \int \frac{dE}{2\pi\Delta_x} \left(h_{iij_1j_2} G_{iij_2j_1}^<(k_z; E) - G_{iij_1j_2}^<(k_z; E) h_{iij_2j_1} \right) \right) \quad (3.68)$$

It is important to note that the current between Source and Drain contacts is not conserved because a part of it can flow through the Gate contact. Only the total current is conserved.

3.2.2 Strength and Weakness

A. Svizhenko and al. describe in [14] a 2D generalization of the formalism presented by R. Lake in [4]. The Green's functions are used to compute carrier and current density for a MOSFET nanotransistor but only for ballistic transport. In this case, the authors of [14] show an efficient algorithm to compute only the desired Green's functions for the evaluation of the current and the carrier density. The problem is that it does not work if interactions are included in the model, which is a strong restriction.

3.3 2D Nanotransistor with Mode Space Method

M. Lundstrom and co-workers apply a two-dimensional quantum mechanical simulation scheme based on nonequilibrium Green's functions to study the behavior of nanoscale transistors[18] as shown in Figure 3.3.

The method consists in an expansion of the Green's functions in coupled mode space: this is equivalent to solve the Schrödinger equation in the z -direction (see Fig. 3.3) and to use the resulting eigenfunction as basis for the Green's function. This method reduces the size of the problem (because instead of discretizing the z -direction with N_z points, a small number of transverse modes are considered)

a rotation of the coordinates occurs: x becomes z , z y , and y x . Hence, the expansion of the Green's functions with pseudo-Wannier functions $\phi_{ij}(xz)$ centered around x_i and z_j yields

$$\begin{aligned} G(11') &= \frac{1}{L_y} \sum_{ii'} \sum_{jj'} \sum_{k_y} \phi_{ij}(xz) G_{ii'jj'}(k_y; tt') \phi_{i'j'}^*(x'z') e^{ik_y(y-y')}, \\ G_{ii'jj'}(k_y; tt') &= \int d\mathbf{r}' \int d\mathbf{r} \phi_{ij}^*(xz) G(11') \phi_{i'j'}(x'z') e^{-ik_y(y-y')}. \end{aligned} \quad (3.69)$$

The equations of motion for the retarded (G^R) and the lesser ($G^<$) Green's functions obtained from equation (2.45) are similar to (3.56) and can be cast into matrix equations

$$\begin{aligned} (\mathbf{E} - \mathbf{H} - \Sigma^R) \mathbf{G}^< &= \Sigma^< \mathbf{G}^A \\ (\mathbf{E} - \mathbf{H} - \Sigma^R) \mathbf{G}^R &= \mathbf{I}, \end{aligned} \quad (3.70)$$

where \mathbf{E} and \mathbf{I} are diagonal $(N_x N_z) \times (N_x N_z)$ matrices and $\mathbf{G}^<$, \mathbf{G}^R , \mathbf{G}^A , Σ^R , and $\Sigma^<$ are full $(N_x N_z) \times (N_x N_z)$ matrices. In fact they are composed of $N_x N_x$ submatrices of size $N_z N_z$, each of them representing a slice in the z -direction. This is important when one considers the Hamiltonian matrix \mathbf{H} whose elements are given by

$$h_{ii'jj'} = \begin{cases} h_{ijj} = t_{jj}^{ii+1} + t_{jj}^{ii-1} + t_{jj+1}^{ii} + t_{jj-1}^{ii} + V_{ij} + \frac{\hbar^2 k_y^2}{2m^* y} & i' = i, j' = j \\ h_{ii\pm 1jj} = -t_{jj}^{ii\pm 1} & i' = i \pm 1, j' = j \\ h_{iijj\pm 1} = -t_{jj\pm 1}^{ii} & i' = i, j' = j \pm 1. \\ 0 & \text{otherwise.} \end{cases}$$

The $t_{jj'}^{ii'}$'s have the following values

$$t_{jj'}^{ii'} = \begin{cases} t_{jj}^{ii\pm 1} = \frac{\hbar^2}{(m_i^{*x} + m_{i\pm 1}^{*x}) \Delta_x^2} & i' = i \pm 1, j' = j, \\ t_{jj\pm 1}^{ii} = \frac{\hbar^2}{(m_j^{*z} + m_{j\pm 1}^{*z}) \Delta_z^2} & i' = i, j' = j \pm 1, \\ 0 & \text{otherwise.} \end{cases} \quad (3.71)$$

By taking into account all these definitions, the Hamiltonian matrix \mathbf{H} can be written in a simple form, where each element is a $N_z N_z$ submatrix

$$\mathbf{H} = \begin{pmatrix} \alpha_1 & \beta_{12} & 0 & \cdots & \cdots \\ \beta_{21} & \alpha_2 & \beta_{23} & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \beta_{N_x-1 N_x-2} & \alpha_{N_x} - \mathbf{1} & \beta_{N_x-1 N_x} \\ 0 & \cdots & 0 & \beta_{N_x N_x-1} & \alpha_{N_x} \end{pmatrix}, \quad (3.72)$$

$$\alpha_{\mathbf{i}} = \begin{pmatrix} h_{ii11} & h_{ii12} & 0 & \cdots & \cdots \\ h_{ii21} & h_{ii22} & h_{ii23} & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & h_{iiN_z-1N_z-2} & h_{iiN_z-1N_z-1} & h_{iiN_z-1N_z} \\ 0 & \cdots & 0 & h_{iiN_zN_z-1} & h_{iiN_zN_z} \end{pmatrix}, \quad (3.73)$$

$$\beta_{\mathbf{i}_1\mathbf{i}_2} = \begin{pmatrix} h_{i_1i_211} & 0 & \cdots & \cdots & \cdots \\ 0 & h_{i_1i_222} & 0 & \cdots & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & h_{i_1i_2N_z-1N_z-1} & 0 \\ 0 & \cdots & \ddots & \ddots & h_{i_1i_2N_zN_z} \end{pmatrix}. \quad (3.74)$$

The idea behind the mode space expansion of the Green's functions is the search of the eigenfunctions $\mathbf{v}_{\mathbf{n}}^{\mathbf{i}}$ (size $N_z \times 1$) and eigenenergies E_n^i of the α 's matrices (n corresponds to the n^{th} mode and i determines its position, i.e. x_i). From the N_z found eigenfunctions $\mathbf{v}_{\mathbf{n}}^{\mathbf{i}}$, only the first N_m modes with small eigenenergies E_n are taken into account, so that one gains a factor $(N_z/N_m)^2$ because the new size of the problem is $(N_x N_m)^2 \times N_{k_y} \times N_E$ instead of $(N_x N_z)^2 \times N_{k_y} \times N_E$. These sizes correspond to the number of unknown Green's functions one is looking for. One has therefore

$$\alpha_{\mathbf{i}} \mathbf{v}_{\mathbf{n}}^{\mathbf{i}} = E_n^i \mathbf{v}_{\mathbf{n}}^{\mathbf{i}} \quad (3.75)$$

and the eigenvectors $\mathbf{v}_{\mathbf{n}}^{\mathbf{i}}$ are used to build the transformation matrix \mathbf{U} whose size is $(N_x N_z) \times (N_m N_x)$

$$\mathbf{U} = \sqrt{\Delta_z} \begin{pmatrix} \mathbf{v}_1^1 & \cdots & \mathbf{v}_{N_m}^1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \mathbf{v}_1^2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \cdots & \vdots & \cdots & \ddots & \vdots & \cdots & \vdots & \cdots \\ 0 & \cdots & 0 & 0 & \cdots & \mathbf{v}_{N_m}^{N_x-1} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \mathbf{v}_1^{N_x} & \cdots & \mathbf{v}_{N_m}^{N_x} \end{pmatrix} \quad (3.76)$$

\mathbf{U} has interesting properties due to the orthogonality of the eigenvectors $\mathbf{v}_{\mathbf{n}}^{\mathbf{i}}$: $\mathbf{U}^T \cdot \mathbf{U} = \mathbf{I}_{N_x N_m \times N_x N_m}$. If one defines now the $N_z \times N_m$ matrix $\mathbf{v}^{\mathbf{i}} = [\mathbf{v}_1^{\mathbf{i}} \mathbf{v}_2^{\mathbf{i}} \cdots \mathbf{v}_{N_m}^{\mathbf{i}}]$, the notation for the matrix \mathbf{U} can be further simplified and becomes

$$\mathbf{U} = \sqrt{\Delta_z} \begin{pmatrix} \mathbf{v}^1 & 0 & \cdots & 0 \\ 0 & \mathbf{v}^2 & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & \ddots & \mathbf{v}^{N_x} \end{pmatrix}. \quad (3.77)$$

In the mode space expansion, the Green's functions do not explicitly depend on the z -coordinates any more but on the confined eigenmode obtained in this direction.

As consequence $G_{ii'jj'}(k_y; tt')$ is transformed into $G_{ii'mm'}(k_y; tt')$ where m and m' run from 1 to N_m and the relation between the Green's function matrix $\mathbf{G}_{\mathbf{rs}}$ in the real space and $\mathbf{G}_{\mathbf{ms}}$ in the mode space is given by

$$\mathbf{G}_{\mathbf{ms}} = \mathbf{U}^T \mathbf{G}_{\mathbf{rs}} \mathbf{U}, \quad \mathbf{G}_{\mathbf{rs}} = \mathbf{U} \mathbf{G}_{\mathbf{ms}} \mathbf{U}^T. \quad (3.78)$$

The second equality results from the eigenmode expansion of the real space Green's function, written in a matrix form. Therefore, if one multiplies equation (3.70) for the retarded Green's function matrix $\mathbf{G}^{\mathbf{R}}$ (the same holds for the lesser) on the left with \mathbf{U}^T and on the right with \mathbf{U} , one obtains

$$\begin{aligned} \mathbf{U}^T (\mathbf{E} - \mathbf{H} - \Sigma^{\mathbf{R}}) \mathbf{G}_{\mathbf{rs}}^{\mathbf{R}} \mathbf{U} &= \mathbf{I}_{N_m N_x \times N_m N_x} \\ \left(\underbrace{\mathbf{U}^T (\mathbf{E} - \mathbf{H}) \mathbf{U}}_{\mathbf{H}_{\mathbf{ms}}} - \underbrace{\mathbf{U}^T \Sigma^{\mathbf{R}} \mathbf{U}}_{\Sigma_{\mathbf{ms}}^{\mathbf{R}}} \right) \mathbf{G}_{\mathbf{ms}}^{\mathbf{R}} &= \mathbf{I}_{N_m N_x \times N_m N_x}. \end{aligned} \quad (3.79)$$

The second part is obtained by replacing $\mathbf{G}_{\mathbf{rs}}^{\mathbf{R}}$ by its mode space expansion given in equation (3.78). It remains to evaluate the mode space form $\mathbf{H}_{\mathbf{ms}}$ of the Hamiltonian and $\Sigma_{\mathbf{ms}}^{\mathbf{R}}$ of the retarded self-energy. $\mathbf{H}_{\mathbf{ms}}$ is evaluated with

$$\mathbf{H}_{\mathbf{ms}} = \begin{pmatrix} \mathbf{E} - \mathbf{E}^1 & -\gamma_{12} & 0 & \cdots & \cdots \\ -\gamma_{21} & \mathbf{E} - \mathbf{E}^2 & -\gamma_{23} & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \gamma_{N_x-1 N_x-2} & \mathbf{E} - \mathbf{E}^{N_x-1} & \gamma_{N_x-1 N_x} \\ 0 & \cdots & 0 & \gamma_{N_x N_x-1} & \mathbf{E} - \mathbf{E}^{N_x} \end{pmatrix} \quad (3.80)$$

where

$$\mathbf{E} = E \times \mathbf{I}_{N_m \times N_m}, \quad \mathbf{E}^i = \begin{pmatrix} \mathbf{E}_1^i & 0 & \cdots & 0 \\ 0 & \mathbf{E}_2^i & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & \ddots & \mathbf{E}_{N_m}^i \end{pmatrix} \quad (3.81)$$

and

$$\gamma_{ij} = \mathbf{v}^i{}^T \beta_{ij} \mathbf{v}^j \quad (3.82)$$

whose size is $N_m \times N_m$. Note that if the effective mass m^{*x} is constant in the z -direction (i.e. no hetero-interface in this direction), then all the elements of the β_{ij} submatrices are identical, and furthermore, if the eigenmodes between two adjacent slices situated at x_i and x_{i+1} are almost the same, then the γ_{ij} submatrices are diagonal. If for simplicity one assumes that γ_{ij} is diagonal without considering the two conditions mentioned above (no hetero-interface in the z -direction, no strong potential variation in the x -direction), then subbands with different energies do not couple and secondly, coupling information of a subband with itself is lost [19].

The transformation from real space to mode space is also required for the self-energies. Normally, the real space self-energy is given by an expression similar to equation (3.69)

$$\Sigma_{ii'jj'}(k_y; tt') = \int d\mathbf{r} \int d\mathbf{r}' \phi_{ij}^*(xz) \Sigma(11') \phi_{i'j'}(x'z') e^{-ik_y(y-y')} \quad (3.83)$$

where, as usual, $\phi_{ij}(xz)$ is a pseudo-Wannier function centered around the point (x_i, z_j) . To represent the real space self-energy in the mode space expansion, it can be very easily proved that the part of the pseudo-Wannier function $\phi_{ij}(xz)$ centered around z_j must be replaced by the eigenmode $v_m^i(z)$ coming from the submatrix α_i situated at x_i . This yields the following expression

$$\Sigma_{ii'mm'}(k_y; tt') = \int d\mathbf{r} \int d\mathbf{r}' \phi_i^*(x) v_m^{*i}(z) \Sigma(11') v_{m'}^{i'}(z') \phi_{i'}(x') e^{-ik_y(y-y')}. \quad (3.84)$$

This concludes the description of the mode space expansion for the Green's functions. Current and carrier density are evaluated with equations (3.64) and (3.68). For that purpose, the mode space Green's function is transformed back to real space.

3.3.2 Strength and Weakness

M. Lundstrom et al. develop in [18] a mode-space expansion of the Green's functions in order to get a 1-dimensional problem instead of a 2- or 3-D one. In that configuration, the discretization of the device in one or two directions is replaced by the eigenmodes obtained in that direction, so that the size of the problem is reduced by a factor $(N_m/N_z)^2$ where N_m is the number of modes taken into account and N_z the number of discretization points in the confined direction. As consequence, a matrix equation of size $(N_x N_m) \times (N_x N_m)$ must be solved $N_E \times N_{k_y}$ times: N_x is the number of points in the transport direction, N_E the number of energy points, and N_{k_y} the number of wavevector points. If the number of confined modes is low, the gain in computer resource is high because one has to solve a quasi 1D problem, where the scattering events can be taken into account rigorously. This is a big advantage in comparison to the method proposed in [14], where only ballistic transport is possible.

However, the mode-space method has some drawbacks: if the submatrices γ_{ij} are assumed diagonal and the confinement potential quickly varies in the transport direction, as described in [19], then coupling informations are lost and the method fails. Furthermore, the mode space expansion is adequate as long a transport direction can be selected and the eigenmode calculated in the transverse directions. If three contacts are present and current can flow either from drain to source or through the gate, i.e. in a direction perpendicular to the main current direction, the eigenmode expansion is no more possible because the system is also open in what should be the confined direction.

As conclusion, the mode-space approach is more efficient than the real-space because it allows the inclusion of accurate scattering mechanisms but fails if certain confinement conditions mentioned above are not fulfilled.

3.4 Quantum Cascade Structures

A. Wacker and S.-C. Lee investigate in [3, 15] the transport and gain properties of quantum cascade (QC) structures using a nonequilibrium Green's functions theory which includes quantum effects beyond a Boltzmann transport description. With this theory, one obtains the nonequilibrium stationary state of QC structures under an applied bias, and hence one determines transport properties, such as the current-voltage characteristics of these devices.

Quantum cascade (QC) structures are grown as a complicated sequence of alternating layers of different semiconductor materials and with varying thickness. This sequence of layers is repeated many times, up to tens or even over a hundred periods. Figure 3.4 shows an example of the conduction band line-up in a QC structure.

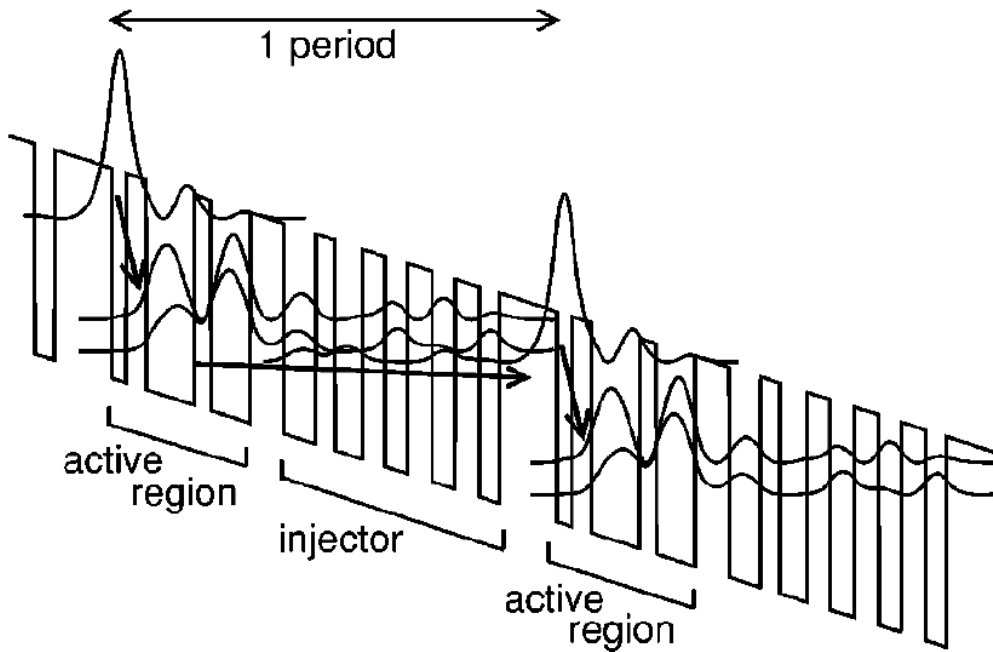


Figure 3.4: Example of the conduction band line-up in a quantum cascade structure with an applied bias. The different Wannier functions of the system are shown.

3.4.1 Model Summary

The QC structure is modeled as a periodic superlattice structure, in which each period contains N_s semiconductor layers with varying thickness. The Hamiltonian H for this system contains two parts, $H = H_0 + H_{scatt}$, where $H_0 = H_{SL} + H_{\mathcal{E}}$ is treated exactly and H_{scatt} as perturbation through self-energies. H_{SL} models the superlattice potential while $H_{\mathcal{E}} = -e\mathcal{E}z$ describes the effects of the electric field \mathcal{E} applied in the growth direction.

3.4.1.1 Bloch States

The Hamiltonian H is expressed in a set of basis states $\psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z) = \frac{e^{j\mathbf{k}\cdot\mathbf{r}}}{\sqrt{A}}\phi^{\nu}(z)$, where the position vector \mathbf{r} and the in-plane wave vector \mathbf{k} are two-dimensional (2D) vectors, z is the growth direction, A the device area, and ν indicates the subband. The $\psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z)$'s are eigenstates of the bare superlattice Hamiltonian H_{SL}

$$\left(-\frac{\hbar^2}{2m^*(z)} \frac{d^2}{dz^2} - \frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} - \frac{\hbar^2}{2m^*} \frac{d^2}{dy^2} + V(z) \right) \psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z) = E^{\nu}(\mathbf{k}) \psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z).$$

Because the superlattice potential is periodic with period d , one has for the potential $V(z+d) = V(z)$ and the wave function must fulfill the periodic boundary condition

$$\psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z+d) = e^{jqd} \psi_{\mathbf{k}}^{\nu}(\mathbf{r}, z), \quad (3.85)$$

where q takes values between $-\frac{\pi}{d}$ and $\frac{\pi}{d}$. This implies that the energy $E^{\nu}(\mathbf{k}, q)$ and the wave function $\psi_{\mathbf{k},q}^{\nu}(\mathbf{r}, z) = \frac{e^{j\mathbf{k}\cdot\mathbf{r}}}{\sqrt{A}}\phi_q^{\nu}(z)$ also depends on q , and that one has minibands in the superlattice structure instead of discrete energy levels. Therefore, the energy minibands can be written as

$$E^{\nu}(\mathbf{k}, q) = E^{\nu} + \sum_{h=1}^{\infty} 2T_h^{\nu} \cos(hdq) + \frac{\hbar^2 k^2}{2m^*}. \quad (3.86)$$

To find the energies and wavefunctions, the transfer matrix method between the first layer of a superlattice period and the first layer of the next period must be applied. The boundary conditions are the continuity of the wave functions, the continuity of the probability current, and the periodicity of the potential. This procedure is well explained in [3].

The Green's functions are proportional to the creation $\hat{\psi}^{\dagger}(\mathbf{r}, t)$ and annihilation $\hat{\psi}(\mathbf{r}, t)$ operators, which will be given by

$$\begin{aligned} \hat{\psi}^{\dagger}(\mathbf{r}, t) &= \sum_{\nu, \mathbf{k}} \int dq \frac{e^{-j\mathbf{k}\cdot\mathbf{r}_{xy}}}{\sqrt{A}} \phi_q^{*\nu}(z) a_{\mathbf{k},q}^{\nu\dagger}(t) \\ \hat{\psi}(\mathbf{r}, t) &= \sum_{\nu, \mathbf{k}} \int dq \frac{e^{j\mathbf{k}\cdot\mathbf{r}_{xy}}}{\sqrt{A}} \phi_q^{\nu}(z) a_{\mathbf{k},q}^{\nu}(t). \end{aligned} \quad (3.87)$$

$a_{\mathbf{k},q}^{\nu\dagger}$ and $a_{\mathbf{k},q}^\nu$ creates and destroys an electron in miniband ν and state (\mathbf{k}, q) , respectively. Furthermore, one has the property

$$\int dz \phi_{q_1}^{*\nu_1}(z) \phi_{q_2}^{\nu_2}(z) = \delta_{\nu_1, \nu_2} \delta(q_1 - q_2). \quad (3.88)$$

The Green's function is then defined in the Heisenberg representation by

$$\begin{aligned} G(11') &= -\frac{i}{\hbar} \langle T \{ \hat{\psi}(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}', t') \} \rangle \\ &= \frac{1}{A} \sum_{\nu_1, \nu_2, \mathbf{k}} \int dq_1 \int dq_2 \phi_{q_1}^{\nu_1}(z) \left(-\frac{i}{\hbar} \right) \langle T \{ a_{\mathbf{k}, q_1}^{\nu_1}(t) a_{\mathbf{k}, q_2}^{\nu_2\dagger}(t') \} \rangle \phi_{q_2}^{*\nu_2}(z') e^{j\mathbf{k}(\mathbf{r}_{\mathbf{xy}} - \mathbf{r}'_{\mathbf{xy}})} \\ &= \frac{1}{A} \sum_{\nu_1, \nu_2, \mathbf{k}} \int dq_1 \int dq_2 \phi_{q_1}^{\nu_1}(z) G^{\nu_1 \nu_2}(\mathbf{k} q_1 q_2; tt') \phi_{q_2}^{*\nu_2}(z') e^{j\mathbf{k}(\mathbf{r}_{\mathbf{xy}} - \mathbf{r}'_{\mathbf{xy}})}. \end{aligned}$$

3.4.1.2 Wannier States

The eigenfunction expansion with Bloch states is not very useful for two reasons: first, there are two integrals over q_1 and q_2 , which are not present in equation (2.25) and secondly, the wave functions $\phi_{q_1}^{\nu_1}(z)$ and $\phi_{q_2}^{*\nu_2}(z')$ are not localized over one period of the superlattice but are delocalized, which induces, for the self-energies as described in section 2.5.3, large matrix elements, like M'_{nn_1} given by equation (2.67). Furthermore the goal is to investigate carrier interactions not only between two energy levels, but also between different superlattice periods, which induces a current through the superlattice. This is numerically possible only when the matrix elements between two wave functions can be neglected, if the wave functions do not belong to the same period, or, if the periods are not adjacent. The solution to meet this requirement consists in transforming the Bloch eigenstates of the superlattice Hamiltonian H_{SL} into Wannier functions centered around one period of the superlattice, as shown in Figure 3.4. This is done with the following rule

$$\begin{aligned} \psi^\nu(z - nd) &= \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} dq e^{-jnqd} \phi_q^\nu(z) \\ \phi_q^\nu(z) &= \sqrt{\frac{d}{2\pi}} \sum_n e^{jnqd} \psi^\nu(z - nd) \end{aligned} \quad (3.89)$$

where $\psi^\nu(z - nd)$ is a Wannier function constructed from the superposition of Bloch eigenstates coming from H_{SL} . It obeys the normalization rule

$$\int dz \psi^{*\nu_1}(z - nd) \psi^{\nu_2}(z - md) = \delta_{\nu_1 \nu_2} \delta_{nm}. \quad (3.90)$$

$\psi^\nu(z - nd)$ is associated with miniband ν and centered around period n . If the wave functions are changed from Bloch $\phi_q^\nu(z)$ to Wannier $\psi^\nu(z - nd)$ states, then the operators $a_{\mathbf{k},q}^{\nu\dagger}$ and $a_{\mathbf{k},q}^\nu$ must also be modified, in order that the position and time

dependent annihilation and creation operators $\hat{\psi}(\mathbf{r}, t)$ and $\hat{\psi}^\dagger(\mathbf{r}, t)$ remain constant. For instance, $\hat{\psi}(\mathbf{r}, t)$ must destroy an electron at place \mathbf{r} and time t

$$\begin{aligned}
\hat{\psi}(\mathbf{r}, t) &= \sum_{\nu, \mathbf{k}} \int dq \frac{e^{j\mathbf{k} \cdot \mathbf{r}_{\mathbf{xy}}}}{\sqrt{A}} \phi_q^\nu(z) a_{\mathbf{k}, q}^\nu(t) \\
&= \sum_{\nu, \mathbf{k}} \sum_n \frac{e^{j\mathbf{k} \cdot \mathbf{r}_{\mathbf{xy}}}}{\sqrt{A}} \psi^\nu(z - nd) a_{\mathbf{k}, n}^\nu(t) \\
\Rightarrow a_{\mathbf{k}, n}^\nu &= \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} dq e^{jnqd} a_{\mathbf{k}, q}^\nu \\
a_{\mathbf{k}, q}^\nu &= \sqrt{\frac{d}{2\pi}} \sum_n e^{-jnqd} a_{\mathbf{k}, n}^\nu
\end{aligned} \tag{3.91}$$

where $a_{\mathbf{k}, n}^\nu$ annihilates an electron situated in period n , miniband ν , and state \mathbf{k} . Inserting these results into the definition of the Green's functions yields

$$\begin{aligned}
G(11') &= -\frac{i}{\hbar} \langle T \{ \hat{\psi}(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}', t') \} \rangle \\
&= \frac{1}{A} \sum_{\nu_1, \nu_2, \mathbf{k}} \sum_{nm} \psi^{\nu_1}(z - nd) \left(-\frac{i}{\hbar} \right) \langle T \{ a_{\mathbf{k}, n}^{\nu_1}(t) a_{\mathbf{k}, m}^{\dagger \nu_2}(t') \} \rangle \psi^{* \nu_2}(z' - md) e^{j\mathbf{k}(\mathbf{r}_{\mathbf{xy}} - \mathbf{r}'_{\mathbf{xy}})} \\
&= \frac{1}{A} \sum_{\nu_1, \nu_2, \mathbf{k}} \sum_{nm} \psi^{\nu_1}(z - nd) G_{nm}^{\nu_1 \nu_2}(\mathbf{k}; tt') \psi^{* \nu_2}(z' - md) e^{j\mathbf{k}(\mathbf{r}_{\mathbf{xy}} - \mathbf{r}'_{\mathbf{xy}})}.
\end{aligned}$$

This equation is similar to (2.25) and enables one to derivate Dyson's equation for the Green's functions. The Wannier expansion of the Green's functions implies that all the matrix element or overlap integrals are computed with Wannier eigenfunctions instead of Bloch or orbital [4, 14] functions. For example, $h_{nm}^{\nu_1 \nu_2}$ from equation (2.45) becomes

$$\begin{aligned}
h_{nm}^{\nu_1 \nu_2} &= \int dz \psi^{\nu_1*}(z - nd) H_0 \psi^{\nu_2}(z - md) \\
&= \int dz \psi^{\nu_1*}(z - nd) H_{SL} \psi^{\nu_2}(z - md) \\
&\quad + \int dz \psi^{\nu_1*}(z - nd) H_{\mathcal{E}} \psi^{\nu_2}(z - md) \\
&= H_{SLnm}^{\nu_1 \nu_2} + H_{\mathcal{E}nm}^{\nu_1 \nu_2} \\
H_{SLnm}^{\nu_1 \nu_2} &= \frac{d}{2\pi} \int dq_1 \int dq_2 \int dz \phi_{q_1}^{* \nu_1}(z) H_{SL} \phi_{q_2}^{\nu_2}(z) e^{jnq_1 d} e^{-jm q_2 d} \\
&= \frac{d}{2\pi} \int dq_1 \int dq_2 E^{\nu_1}(0, q_1) \delta_{\nu_1, \nu_2} \delta(q_1 - q_2) e^{j(n-m)q_2 d} \\
&= \frac{d}{2\pi} \int dq E^{\nu_1}(0, q) \delta_{\nu_1, \nu_2} e^{j(n-m)qd} \\
&= \delta_{\nu_1, \nu_2} \cdot \begin{cases} E^{\nu_1} & m = n, \\ T_h^{\nu_1} & m = n \pm h, \quad h \geq 1 \end{cases}
\end{aligned}$$

$$\begin{aligned}
H_{\mathcal{E}nm}^{\nu_1\nu_2} &= - \int dz \psi^{\nu_1*}(z - nd) e\mathcal{E} z \psi^{\nu_2}(z - md) \\
&= - \int dz \psi^{\nu_1*}(z - (n - m)d) e\mathcal{E}(z + md) \psi^{\nu_2}(z) \\
&= -e\mathcal{E} \cdot \begin{cases} R_0^{\nu_1\nu_2} + nd\delta_{\nu_1,\nu_2}, & m = n \\ R_h^{\nu_1\nu_2}, & m = n \pm h \quad h \geq 1 \end{cases} \\
R_h^{\nu_1\nu_2} &= \int dz \psi^{\nu_1*}(z - hd) z \psi^{\nu_2}(z).
\end{aligned} \tag{3.92}$$

These are all the elements required to compute $h_{nm}^{\nu_1\nu_2}$. The self-energies are calculated as presented in section 2.5.3, but with Wannier functions for the matrix elements. Then, Dyson's equations for the retarded and the lesser Green's functions for stationary state are given by

$$\begin{aligned}
EG_{nm}^{<\nu_1\nu_2}(\mathbf{k}; E) - \sum_{l\nu_3} h_{nl}^{\nu_1\nu_3} G_{lm}^{<\nu_3\nu_2}(\mathbf{k}; E) &= \sum_{l\nu_3} \Sigma_{nl}^{R\nu_1\nu_3}(\mathbf{k}; E) G_{lm}^{<\nu_3\nu_2}(\mathbf{k}; E) + \\
&\quad \sum_{l\nu_3} \Sigma_{nl}^{<\nu_1\nu_3}(\mathbf{k}; E) G_{lm}^{A\nu_3\nu_2}(\mathbf{k}; E) \\
EG_{nm}^{R\nu_1\nu_2}(\mathbf{k}; E) - \sum_{l\nu_3} h_{nl}^{\nu_1\nu_3} G_{lm}^{R\nu_3\nu_2}(\mathbf{k}; E) &= \delta_{nm} \delta_{\nu_1\nu_2} + \sum_{l\nu_3} \Sigma_{nl}^{R\nu_1\nu_3}(\mathbf{k}; E) G_{lm}^{R\nu_3\nu_2}(\mathbf{k}; E).
\end{aligned} \tag{3.93}$$

The advantage of the Wannier functions is that they are localized, in this case over a superlattice period, so that the overlap integrals, and therefore the self-energies Σ_{nl} and the Hamiltonian h_{nl} get smaller as the difference $|l - n|$ increases. A procedure to obtain as localized as possible Wannier functions is explained in [15] (the position operator \hat{z} is expressed in the Wannier basis obtained from equation (3.90), then diagonalized, and the resulting eigenfunctions give the required set of Wannier functions). Hence one can assume that Σ_{nl} and h_{nl} vanish if $l \notin [n - 1, n, n + 1]$. This simplifies the matrix equation (3.93). For example, the equation for the retarded Green's functions becomes

$$\begin{aligned}
&\sum_{\nu_3} \left\{ [(E - E^{\nu_1}(\mathbf{k}, 0) + ne\mathcal{E}d) \delta_{\nu_1\nu_3} + e\mathcal{E}R_0^{\nu_3}] G_{nm}^{R\nu_3\nu_2} - \right. \\
&\left. (T_1^{\nu_1} \delta_{\nu_1\nu_3} - e\mathcal{E}R_1^{\nu_1\nu_3}) (G_{n+1m}^{R\nu_3\nu_2} + G_{n-1m}^{R\nu_3\nu_2}) \right\} = \delta_{nm} \delta_{\nu_1\nu_2} + \sum_{\nu_3, \pm} \Sigma_{nn\pm 1}^{R\nu_1\nu_3} G_{n\pm 1m}^{R\nu_3\nu_2}.
\end{aligned}$$

The boundary conditions must be defined, so that one can solve the system of equations given in (3.93). Because of the periodicity of the structure, one has

$$G_{nm}^{\nu_1\nu_2}(\mathbf{k}; E) = G_{n-1m-1}^{\nu_1\nu_2}(\mathbf{k}; E + e\mathcal{E}d). \tag{3.94}$$

All the conditions are fulfilled to solve the system of equations. One considers the following example: a superlattice structure has nine different minibands below the conduction-band offset and one above (the indices ν run therefore from 1 to 10).

The Green's functions of one period are only coupled to themselves, and the Green's functions of the preceding and following periods. Through the boundary conditions and the self-energies, Green's functions of different energies and wave vector are coupled. Thus, if there are N_E energy points and N_k wavevector points, the number of Green's functions to be found is $(3 \times 10)^2 \times N_E \times N_k$.

As in the previously described applications, carrier-carrier interactions are taken into account on a mean-field level, i.e. Poisson's equation must be solved self-consistently with the Green's functions.

3.4.1.3 Carrier and Current Density

As soon as the Green's functions have been calculated, the quantum transport problem can be solved by evaluating the carrier and current density. For the carrier density, one obtains

$$n(z) = -\frac{i}{A} \sum_{\mathbf{k}_t, \sigma} \sum_{nm} \sum_{\nu_1 \nu_2} \int \frac{dE}{2\pi} G_{nm}^{<\nu_1 \nu_2}(\mathbf{k}_t; E) \psi^{\nu_1}(z - nd) \psi^{*\nu_2}(z - md). \quad (3.95)$$

The calculation of the current density is more complicated than for the resonant tunneling device [4] or for the nanoscale MOSFET [14], because interactions are present everywhere. The current density is therefore given by an adapted equation

$$J = \frac{e}{V} \langle \hat{v} \rangle = \frac{e}{V} \left\langle \frac{d}{dt} \hat{z} \right\rangle \quad (3.96)$$

where \hat{v} is the velocity and \hat{z} the position operator

$$\begin{aligned} \hat{z} &= \sum_{nm} \sum_{\nu_1 \nu_2} \sum_{\mathbf{k} \sigma} z_{nm}^{\nu_1 \nu_2} a_{\mathbf{k}, n}^{\dagger \nu_1} a_{\mathbf{k}, m}^{\nu_2} \\ &= \sum_{nm} \sum_{\nu_1 \nu_2} \sum_{\mathbf{k} \sigma} \int dz \psi^{*\nu_1}(z - nd) z \psi^{\nu_2}(z - md) a_{\mathbf{k}, n}^{\dagger \nu_1} a_{\mathbf{k}, m}^{\nu_2}. \end{aligned} \quad (3.97)$$

The current density can then be written as

$$\begin{aligned} J &= -i\hbar \frac{e}{V} \sum_{nm} \sum_{\nu_1 \nu_2} \sum_{\mathbf{k} \sigma} z_{nm}^{\nu_1 \nu_2} \lim_{t' \rightarrow t} \left(\frac{d}{dt} + \frac{d}{dt'} \right) G_{mn}^{\nu_2 \nu_1}(\mathbf{k}; tt') \\ &= -\frac{e}{V} \sum_{nml} \sum_{\nu_1 \nu_2 \nu_3} \sum_{\mathbf{k} \sigma} z_{nm}^{\nu_1 \nu_2} \left\{ (h_{ml}^{\nu_2 \nu_3} G_{ln}^{<\nu_3 \nu_1}(\mathbf{k}_t; tt) - G_{ml}^{<\nu_2 \nu_3}(\mathbf{k}_t; tt) h_{ln}^{\nu_3 \nu_1}) + \right. \\ &\quad \left. \int dt_2 \left(\left[\Sigma_{ml}^{R\nu_2 \nu_3}(\mathbf{k}_t; tt_2) G_{ln}^{<\nu_3 \nu_1}(\mathbf{k}_t; t_2 t) + \Sigma_{ml}^{<\nu_2 \nu_3}(\mathbf{k}_t; tt_2) G_{ln}^{A\nu_3 \nu_1}(\mathbf{k}_t; t_2 t) \right] - \right. \right. \\ &\quad \left. \left. \left[G_{ml}^{R\nu_2 \nu_3}(\mathbf{k}_t; tt_2) \Sigma_{ln}^{<\nu_3 \nu_1}(\mathbf{k}_t; t_2 t) + G_{ml}^{<\nu_2 \nu_3}(\mathbf{k}_t; tt_2) \Sigma_{ln}^{A\nu_3 \nu_1}(\mathbf{k}_t; t_2 t) \right] \right) \right\} \\ &= -\frac{e}{\hbar V} \sum_{nml} \sum_{\nu_1 \nu_2 \nu_3} \sum_{\mathbf{k} \sigma} \int \frac{dE}{2\pi} \left\{ (z_{nm}^{\nu_1 \nu_2} h_{ml}^{\nu_2 \nu_3} - h_{nm}^{\nu_1 \nu_2} z_{ml}^{\nu_2 \nu_3}) G_{ln}^{<\nu_3 \nu_1}(\mathbf{k}_t; E) + \right. \\ &\quad \left. z_{nm}^{\nu_1 \nu_2} \left(\Sigma_{ml}^{R\nu_2 \nu_3}(\mathbf{k}_t; E) G_{ln}^{<\nu_3 \nu_1}(\mathbf{k}_t; E) + \Sigma_{ml}^{<\nu_2 \nu_3}(\mathbf{k}_t; E) G_{ln}^{A\nu_3 \nu_1}(\mathbf{k}_t; E) \right) - \right. \end{aligned}$$

$$z_{nm}^{\nu_1\nu_2} \left(G_{ml}^{R\nu_2\nu_3}(\mathbf{k}_t; E) \Sigma_{ln}^{<\nu_3\nu_1}(\mathbf{k}_t; E) + G_{ml}^{<\nu_2\nu_3}(\mathbf{k}_t; E) \Sigma_{ln}^{A\nu_3\nu_1}(\mathbf{k}_t; E) \right) \}. \quad (3.98)$$

This equation looks like (2.95), but has some form differences due to the position operator \hat{z} . However, the equivalence of both equations can be proved, if one carefully expands (3.98). The current density has two contributions, one from H_0 , J_0 which corresponds to the first line of the last equality in equation (3.98) and one from the interaction Hamiltonian H_{scatt} , J_{scatt} corresponding to the two last lines of (3.98).

3.4.1.4 Gain Spectra

In Wacker's paper [15], a way to calculate optical gain from the Green's function is derived. Since it is not the purpose of this work to calculate gain and absorption spectra, the subject will not be treated here, but many details are given in [15] and the references therein.

3.4.2 Strength and Weakness

A. Wacker and S.-C. Lee use the nonequilibrium Green's function theory to solve quantum transport in quantum cascade structures. The Green's functions are expanded into Wannier states localized over one period of the superlattice structure. Interactions are only possible between states belonging to the same period or to two adjacent periods. This is very efficient to calculate current and carrier density, but this method does not allow to have interactions between two quantum wells or between two points in the same quantum well. A period in the superlattice structure must be viewed as a single element, being able to interact with other elements. This is surely a weakness of the method, but at the same time it makes the numerical problem solvable.

The interaction mechanisms which are taken into account in [15] are carrier-phonon (optical and acoustic), interface roughness, impurity, and carrier-carrier scattering on a mean-field level (Poisson's equation). To compute the corresponding self-energies, a summation over the 2D wave vector \mathbf{k}_t must be accomplished. This summation is transformed into an integral over an angle θ and over the norm k of the wave vector. To simplify the numeric, the terms which should be integrated over the angle θ are pushed out of the integral and a mean value is taken. Detailed explanations of this method are presented in [15]. The advantage of this procedure is a huge gain of time, but it causes loss of accuracy.

3.5 Conclusion

In this chapter, four different applications of the nonequilibrium Green's function theory were shown to compute 1D or 2D nanostructures. Once the equations to solve a problem are found, including the boundary conditions, the difficulty resides

in the numerical evaluation of them. For ballistic transport, i.e. without carrier interactions, efficient algorithms can be found to obtain current and carrier density. However, as soon as scattering mechanisms are present, the computational burden explodes to run a simulation. To avoid such a problem, simplifications are possible, either by truncating the self-consistent procedure between Green's functions and self-energies [4] or by using localized eigenfunctions, like Wannier functions centered on a period of a superlattice or on a quantum well [15], which reduce the number of points needed to obtain accurate results.

A 3D derivation of Dyson's equation for a quantum dot or for other complicated nanostructures is straightforward, but the numerical implementation is hard. Ballistic transport will be possible within reasonable simulation times, but the inclusion of scattering mechanisms does not seem to be possible, except if a good simplification algorithm is found as in [18].

Appendix A

Interaction Representation

A.1 Schrödinger Picture

In the Schrödinger picture, the operators O_S are time-independent. The time-dependence is contained in the wave functions $|\Psi_S(t)\rangle$, obtained from the Schrödinger equation. The time-independent Hamilton operator $H = H_0 + V$ has a non-interacting part H_0 , whose eigenvalues and eigenvectors can be solved exactly, and a perturbation part V . One has therefore

$$i\hbar \frac{d}{dt} |\Psi_S(t)\rangle = H |\Psi_S(t)\rangle \quad (\text{A.1})$$

with the formal solution

$$|\Psi_S(t)\rangle = e^{-iHt/\hbar} |\Psi_S(0)\rangle = e^{-iHt/\hbar} |\Psi_0\rangle. \quad (\text{A.2})$$

As consequence, the wave functions are time-dependent.

A.2 Heisenberg Picture

It is possible to solve the quantum mechanical problem differently, resulting in the same answers, but using methods that look quite different. The Heisenberg representation has the following properties:

- time-independent wave functions
- time-dependent operator.

The Heisenberg wave functions are given by

$$\begin{aligned} |\Psi_H(t)\rangle &= e^{iHt/\hbar} |\Psi_S(t)\rangle \\ &= |\Psi_H(0)\rangle = |\Psi_0\rangle \end{aligned} \quad (\text{A.3})$$

because

$$\frac{d}{dt} |\Psi_H(t)\rangle = \frac{i}{\hbar} H e^{iHt/\hbar} |\Psi_S(t)\rangle + e^{iHt/\hbar} \frac{d}{dt} |\Psi_S(t)\rangle = 0. \quad (\text{A.4})$$

In order to get the same matrix elements as in the Schrödinger representation, the Heisenberg operators are defined as follow

$$O_H(t) = e^{iHt/\hbar} O_S e^{-iHt/\hbar} \quad (\text{A.5})$$

which corresponds to a time evolution according to the new equation of motion

$$i\hbar \frac{d}{dt} O_H(t) = [O_H(t), H]. \quad (\text{A.6})$$

A.3 Interaction Picture

A.3.1 Definition

In the interaction representation, both the wave functions and the operators are time dependent. This is achieved by taking V , the interaction part of H , as a perturbation. Then the time dependences are given by

$$\begin{aligned} |\Psi_I(t)\rangle &= e^{iH_0 t/\hbar} |\Psi_S(t)\rangle \\ &= e^{iH_0 t/\hbar} e^{-iHt/\hbar} |\Psi_0\rangle \\ &= U_I(t) |\Psi_0\rangle \end{aligned} \quad (\text{A.7})$$

for the wave function and

$$O_I(t) = e^{iH_0 t/\hbar} O_S e^{-iH_0 t/\hbar} \quad (\text{A.8})$$

for the operators whose time evolution is governed by the unperturbed Hamiltonian H_0

$$i\hbar \frac{d}{dt} O_I(t) = [O_I(t), H_0]. \quad (\text{A.9})$$

Putting everything together, it is possible to calculate the time evolution of the wave function,

$$i\hbar \frac{d}{dt} |\Psi_I(t)\rangle = V_I(t) |\Psi_I(t)\rangle \quad (\text{A.10})$$

and of the development operator $U_I(t) = e^{iH_0 t/\hbar} e^{-iHt/\hbar}$ with $U_I(0) = 1$, which obeys the following differential equation

$$i\hbar \frac{d}{dt} U_I(t) = V_I(t) U_I(t). \quad (\text{A.11})$$

Integrating both sides of the equation with respect to time t yields, with the initial condition $U_I(0) = 1$

$$U_I(t) - U_I(0) = -\frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) U_I(t_1) \quad (\text{A.12})$$

or

$$U_I(t) = 1 - \frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) U_I(t_1). \quad (\text{A.13})$$

If this equation is repeatedly iterated, one gets

$$\begin{aligned} U_I(t) &= 1 - \frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) + \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V_I(t_1) V_I(t_2) + \\ &\quad \cdots + \left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n V_I(t_1) V_I(t_2) \cdots V_I(t_n) \\ &= \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n V_I(t_1) V_I(t_2) \cdots V_I(t_n). \end{aligned}$$

With the help of the chronological time ordering operator T^c defined in equation (1.2), the expression for $U_I(t)$ can be simplified [5]:

$$\begin{aligned} U_I(t) &= 1 + \sum_{n=1}^{\infty} \left(\frac{-i/\hbar}{n!}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n T^c \{V_I(t_1) V_I(t_2) \cdots V_I(t_n)\} \\ &= T^c \left\{ \exp \left(-\frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) \right) \right\}. \end{aligned} \quad (\text{A.14})$$

For the inverse operator $U_I^{-1}(t)$, the following equation has to be solved

$$-i\hbar \frac{d}{dt} U_I^{-1}(t) = U_I^{-1}(t) V_I(t) \quad (\text{A.15})$$

with the solution

$$\begin{aligned} U_I^{-1}(t) &= 1 + \sum_{n=1}^{\infty} \left(\frac{i/\hbar}{n!}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n T^a \{V_I(t_1) V_I(t_2) \cdots V_I(t_n)\} \\ &= T^a \left\{ \exp \left(\frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) \right) \right\} \\ &= U_I^\dagger(t). \end{aligned} \quad (\text{A.16})$$

T^a represents the anti-chronological time-ordering operator. If A and B are two general operators, this yields

$$T^a \{A(t) B(t')\} = \theta(t - t') B(t') A(t) + \theta(t' - t) A(t) B(t'), \quad (\text{A.17})$$

but if they are Fermion field operators

$$T^a \{A(t) B(t')\} = \theta(t - t') B(t') A(t) - \theta(t' - t) A(t) B(t'). \quad (\text{A.18})$$

A.3.2 S Matrix

The time development operator $U_I(t)$ takes the wave function from zero time to the time t . A more general operator $S(t, t')$ which takes the wave function from t' to t can be introduced

$$\begin{aligned} |\Psi_I(t)\rangle &= S(t, t')|\Psi_I(t')\rangle \\ &= U_I(t)U_I^\dagger(t')|\Psi_I(t')\rangle \end{aligned} \quad (\text{A.19})$$

with the following properties:

- $S(t, t) = 1$
- $S^\dagger(t, t') = S(t', t)$ because $U_I(t)$ is a unitary operator
- $S(t, t')S(t', t'') = S(t, t'')$
- $S(t, t')$ can be expressed as a time-ordered operator,

$$i\hbar \frac{d}{dt} S(t, t') = V_I(t)S(t, t') \quad (\text{A.20})$$

which has the solution

$$S(t, t') = T\left\{\exp\left(-\frac{i}{\hbar} \int_{t'}^t dt_1 V_I(t_1)\right)\right\}. \quad (\text{A.21})$$

If $t > t'$, T is the chronological time-ordering operator T^c , otherwise, the anti-chronological one T^a .

A.4 Usual Relations between Pictures

The relations between matrix elements in the Heisenberg picture like the Green's functions and the interaction picture are derived

$$\begin{aligned} \langle O_H(t) \rangle &= \langle e^{iHt/\hbar} O_S e^{-iHt/\hbar} \rangle \\ &= \langle e^{iHt/\hbar} e^{-iH_0 t/\hbar} O_I(t) e^{iH_0 t/\hbar} e^{-iHt/\hbar} \rangle. \end{aligned} \quad (\text{A.22})$$

With equations (A.8), this relation is rewritten as

$$\begin{aligned} \langle O_H(t) \rangle &= \langle U_I^\dagger(t) O_I(t) U_I(t) \rangle \\ &= \langle S^\dagger(t, 0) O_I(t) S(t, 0) \rangle \\ &= \langle S(0, t) O_I(t) S(t, 0) \rangle. \end{aligned} \quad (\text{A.23})$$

If the reference time is taken at t_o instead of 0, the relation between the Heisenberg and the interaction picture becomes

$$\langle O_H(t) \rangle = \langle S(t_o, t) O_I(t) S(t, t_o) \rangle. \quad (\text{A.24})$$

As it will be seen later, the Wick's decomposition holds exactly and therefore can only be applied for operators in the interaction picture.

Appendix B

Interaction Representation for Imaginary Times

As in Appendix A, a straightforward procedure to treat the perturbation V of H given by $H = H_0 + V$ will be derived in case of imaginary times.

B.1 Pseudo Schrödinger Picture

The starting point is the equation for the density matrix ρ present in the thermodynamic average of equation (1.10) for example

$$\rho_S = e^{-\beta(H-\mu N)}. \quad (\text{B.1})$$

The density operator ρ_S obeys the following differential equation

$$\frac{d\rho_S}{d\beta} = -(H - \mu N)\rho_S. \quad (\text{B.2})$$

B.2 Pseudo Heisenberg Picture

The pseudo Heisenberg density operator ρ_H is given by:

$$\rho_H = e^{\beta(H-\mu N)}\rho_S \quad (\text{B.3})$$

which implies that $\frac{d\rho_H}{d\beta} = 0$ and the operators in this representation become:

$$O_H(\tau) = e^{\tau(H-\mu N)/\hbar} O_S e^{-\tau(H-\mu N)/\hbar}. \quad (\text{B.4})$$

B.3 Pseudo Interaction Picture

In this representation, the density operator ρ_I is given by

$$\rho_I = e^{\beta(H_0-\mu N)}\rho_S = e^{\beta(H_0-\mu N)}e^{\beta(H-\mu N)} \quad (\text{B.5})$$

and the operators in the pseudo-interaction picture obey the following equation

$$O_I(\tau) = e^{\tau(H_0 - \mu N)/\hbar} O_S e^{-\tau(H_0 - \mu N)/\hbar}. \quad (\text{B.6})$$

To recall a formalism similar to the one described in Appendix A, a time development operator $\mathcal{U}(\tau)$ is introduced with

$$\mathcal{U}(\tau) = \rho_I \left(\beta - > \frac{\tau}{\hbar} \right). \quad (\text{B.7})$$

Then, $\mathcal{U}(\tau)$ is governed by a differential equation very similar to (A.11)

$$\hbar \frac{d}{d\tau} \mathcal{U}_I(\tau) = V_I(\tau) \mathcal{U}_I(\tau). \quad (\text{B.8})$$

Integrating both sides of the equation with respect to the imaginary time τ yields

$$\mathcal{U}_I(\tau) - \mathcal{U}_I(0) = -\frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \mathcal{U}_I(\tau_1) \quad (\text{B.9})$$

or

$$\mathcal{U}_I(\tau) = 1 - \frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \mathcal{U}_I(\tau_1). \quad (\text{B.10})$$

If this equation is repeatedly iterated, one obtains

$$\begin{aligned} \mathcal{U}_I(\tau) &= 1 - \frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) + \left(\frac{-1}{\hbar} \right)^2 \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n) \\ &= \sum_{n=0}^{\infty} \left(\frac{-1}{\hbar} \right)^n \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n). \end{aligned}$$

With the help of the imaginary time-order operator T_τ , the expression for $\mathcal{U}_I(\tau)$ can be simplified [5]

$$\begin{aligned} \mathcal{U}_I(\tau) &= 1 + \sum_{n=1}^{\infty} \left(\frac{-1/\hbar}{n!} \right)^n \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 \cdots \int_0^\tau d\tau_n T_\tau \{ V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n) \} \\ &= T_\tau \left\{ \exp \left(-\frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \right) \right\}. \end{aligned} \quad (\text{B.11})$$

B.3.1 \mathcal{S} Matrix

The time development operator $\mathcal{U}_I(\tau)$ describes an evolution from zero time to the imaginary time τ . A more general operator $\mathcal{S}(\tau, \tau')$ that takes the wave function from τ' to τ can be introduced and has the following important properties:

- $\mathcal{S}(\tau, \tau) = 1$
- $\mathcal{S}(\tau, \tau') \mathcal{S}(\tau', \tau'') = \mathcal{S}(\tau, \tau'')$

- $\mathcal{S}(\tau, \tau')$ can be expressed as a time-ordered operator,

$$\hbar \frac{d}{d\tau} \mathcal{S}(\tau, \tau') = V_I(\tau) \mathcal{S}(\tau, \tau') \quad (\text{B.12})$$

which has the solution

$$\mathcal{S}(\tau, \tau') = T_{\tau} \left\{ \exp \left(-\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau_1 V_I(\tau_1) \right) \right\}. \quad (\text{B.13})$$

Appendix C

External Perturbation

If an external perturbation $H^{ext}(t)$ is applied to an equilibrium system, the total Hamiltonian $\mathcal{H}(t)$ becomes

$$\mathcal{H}(t) = H_0 + V + H^{ext}(t) = H + H^{ext}(t) \quad (C.1)$$

where H_0 , V and $H^{ext}(t)$ are given by equations (1.45) and (2.1) for example. The time-dependent Schrödinger equation takes then the form

$$\begin{aligned} i\hbar \frac{d}{dt} |\psi_S(t)\rangle &= \mathcal{H}(t) |\psi_S(t)\rangle \\ &= (H + H^{ext}(t)) |\psi_S(t)\rangle. \end{aligned} \quad (C.2)$$

The time evolution operator $U_S(t, t_0)$ with $|\psi(t)\rangle = U_S(t, t_0) |\psi_S(t_0)\rangle$ obeys the same Schrödinger equation as $|\psi_S(t)\rangle$. One has therefore

$$i\hbar \frac{d}{dt} U_S(t, t_0) = \mathcal{H}(t) U_S(t, t_0). \quad (C.3)$$

To solve this equation, it is convenient to separate the influence of H and $H^{ext}(t)$. This is possible with the ansatz

$$U_S(t, t_0) = e^{-iH(t-t_0)/\hbar} S_H^{ext}(t, t_0). \quad (C.4)$$

For $S_H^{ext}(t, t_0)$ follows a differential equation very similar to (A.11)

$$\begin{aligned} i\hbar \frac{d}{dt} S_H^{ext}(t, t_0) &= e^{iH(t-t_0)/\hbar} H^{ext}(t) e^{-iH(t-t_0)/\hbar} S_H^{ext}(t, t_0) \\ &= H_H^{ext}(t) S_H^{ext}(t, t_0). \end{aligned} \quad (C.5)$$

The solution is obtained by repeated iteration of the equation

$$S_H^{ext}(t, t_0) = T \left\{ \exp \left(-\frac{i}{\hbar} \int_{t_0}^t dt_1 H_H^{ext}(t_1) \right) \right\}. \quad (C.6)$$

As t_0 is the initial time of the system, t is always larger than t_0 and the time operator T corresponds to the chronological time-ordering operator T_c . $S_H^{ext}(t, t_0)$ has the same properties as the S matrix introduced in Appendix A.

C.1 Heisenberg Representation

A wave function $|\psi_{\mathcal{H}}(t)\rangle$ and an operator $O_{\mathcal{H}}(t)$ in the Heisenberg representation with respect to \mathcal{H} are introduced

$$\begin{aligned} |\psi_{\mathcal{H}}(t)\rangle &= U_S^{-1}(t, t_0) |\psi_S(t_0)\rangle \\ O_{\mathcal{H}}(t) &= U_S^{-1}(t, t_0) O_S U_S(t, t_0). \end{aligned} \quad (\text{C.7})$$

Therefore, one obtains for the expectation value $\langle O_{\mathcal{H}}(t) \rangle$

$$\begin{aligned} \langle O_{\mathcal{H}}(t) \rangle &= \langle U_S^{-1}(t, t_0) O_S U_S(t, t_0) \rangle \\ &= \langle S_H^{ext-1}(t, t_0) e^{iH(t-t_0)/\hbar} O_S e^{-iH(t-t_0)/\hbar} S_H^{ext}(t, t_0) \rangle \\ &= \langle S_H^{ext}(t_0, t) O_H(t) S_H^{ext}(t, t_0) \rangle. \end{aligned} \quad (\text{C.8})$$

C.2 Application to Nonequilibrium Green's Functions

The nonequilibrium Green's functions $G(x, t; x', t')$ in the presence of an external perturbation $H^{ext}(t)$ included in the Hamiltonian $\mathcal{H}(t)$ are defined by

$$G(x, t; x', t') = -\frac{i}{\hbar} \langle T \{ \hat{\psi}_{\mathcal{H}}(x, t) \hat{\psi}_{\mathcal{H}}^{\dagger}(x', t') \} \rangle. \quad (\text{C.9})$$

Changing the picture reference for the operators given in the Heisenberg representation from $\mathcal{H}(t)$ to H yields

$$\begin{aligned} G(x, t; x', t') &= -\frac{i}{\hbar} \langle T \{ S(t_0, t) \hat{\psi}_H(x, t) S(t, t_0) S(t_0, t') \hat{\psi}_H^{\dagger}(x', t') S(t', t_0) \} \rangle \\ &= -\frac{i}{\hbar} \frac{\langle T \{ S(t_0, t) \hat{\psi}_H(x, t) S(t, t') \hat{\psi}_H^{\dagger}(x', t') S(t', t_0) \} \rangle}{\langle S(t_0, t_0) \rangle} \\ &= -\frac{i}{\hbar} \frac{\langle T \{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(x, t) \hat{\psi}_H^{\dagger}(x', t') \} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \end{aligned} \quad (\text{C.10})$$

where $S_H^{ext}(t_0, t_0)$ contains an integral along a time contour as the one of figure 1.1, the denominator $\langle S_H^{ext}(t_0, t_0) \rangle$ is equal to 1, but will be useful in the variational derivation of the self-energies (Hartree term originated from the derivative of the denominator), and

$$S_H^{ext}(t_0, t_0) = T \left\{ \exp \left(-\frac{i}{\hbar} \oint_{t_0}^{t_0} dt_1 H_H^{ext}(t_1) \right) \right\} \quad (\text{C.11})$$

Appendix D

Wick's Decomposition

Wick's decomposition allows a perturbation expansion of the Green's functions of all types. It always holds for zero-temperature Green's functions and only under certain conditions, if the temperature is different from zero (in this case the expectation value of the operator O , which is the product of field-operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ becomes $\langle O \rangle = \frac{\text{Tr}\{\rho O\}}{\text{Tr}\{\rho\}}$) [11]:

- the density operator ρ must be of the form

$$\rho = \exp(\mathcal{A}) \quad (\text{D.1})$$

with \mathcal{A} being a 1-particle operator like $\mathcal{A} = \sum \mathcal{A}_j c_j^\dagger c_j$. Therefore, if the system possesses initial correlations, this is not satisfied and the expectation value $\langle O \rangle$ must be first modified (Appendix H).

- if the Hamiltonian H is given by $H = H_0 + V$, the field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ included in the operator O must be given in the interaction picture (Appendix A), i.e. their time evolution must only contain H_0 . V is treated as a perturbation.

If these conditions are fulfilled, Wick's theorem states that the expectation values of products of field operators $\hat{\psi}_I$ and $\hat{\psi}_I^\dagger$ (many-particle Green's functions) factorize into expectation values of pairs of operators (free 1-particle Green's functions).

$$\begin{aligned} \langle T\{A_I B_I \cdots Y_I Z_I\} \rangle &= A_I B_I \cdots Y_I Z_I + A_I B_I \cdots Y_I Z_I + \cdots \\ &= \text{sum over all possible contracted products} \end{aligned} \quad (\text{D.2})$$

where the contraction

$$A_I B_I = \langle T\{A_I B_I\} \rangle \quad (\text{D.3})$$

and T is the contour-order operator. Further terms called "normal order products of operators" appear in the last equations but their expectation values vanish. Hence they are omitted.

Each time a Fermion operator is displaced in order to bring a pair of contracted operators side by side, the total expectation value must be multiplied by a minus sign. A proof for Wick's theorem is given in [10] for zero- and non-zero- temperature expectation values for equilibrium situations and in [11] for nonequilibrium ones. Before going through an example, the contraction $A_I B_I$ has to be considered. If both A_I and B_I are annihilation operators or creation operators, the contraction $A_I B_I$ disappears, otherwise one obtains an expression proportional to the free Green's function G_0 which is equal to the Green's function G when the interaction part V is set to zero

$$A_I(x_1, t_1) B_I(x_2, t_2) = i\hbar G_0(x_1, t_1; x_2, t_2) \quad (\text{D.4})$$

if A_I is the annihilation operator and B_I the creation operator. In the opposite case, one has

$$A_I(x_1, t_1) B_I(x_2, t_2) = i\hbar G_0(x_2, t_2; x_1, t_1). \quad (\text{D.5})$$

There is no imaginary factor i for Matsubara Green's functions. As an example, V will describe the carrier-carrier scattering. One has the following interaction potential

$$V = \frac{1}{2} \int dx_1 \int dx_2 \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) V(x_1 - x_2) \hat{\psi}(x_2) \hat{\psi}(x_1). \quad (\text{D.6})$$

In each kind of Green's functions (equilibrium or nonequilibrium, zero or finite temperature), there is a term of the form

$$\langle T \{ \exp \left(-\frac{i}{\hbar} \int dt_1 V_I(t_1) \right) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle$$

in the numerator, where the limits of the time integral $\int dt_1$ and the averaging method $\langle \rangle$ depend on the considered Green's function. Expanding the exponential function, the first term is trivial and is equal to the free Green's function

$$F_N^{(0)} = \langle T \{ \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle = i\hbar G_0(x, t; x', t'). \quad (\text{D.7})$$

Therefore, the second numerator term will be studied, corresponding to $n = 1$ in equation (A.14)

$$\begin{aligned} F_N^{(1)} &= \langle T \{ -\frac{i}{\hbar} \int dt_1 V_I(t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle \\ &= -\frac{i}{\hbar} \frac{1}{2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \cdot \\ &\quad \langle T \{ \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle. \end{aligned} \quad (\text{D.8})$$

There are six non-vanishing possibilities to contract equation (D.8) with the Wick's theorem

$$\begin{aligned}
F_N^{(1)} = & -\frac{i}{\hbar} \frac{1}{2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \\
& \times [\hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') + \\
& \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') + \\
& \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') + \\
& \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') + \\
& \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') + \\
& \hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I^\dagger(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_1, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t')] . \quad (D.9)
\end{aligned}$$

Replacing the contraction products by free Green's functions G_0 (no i for the Matsubara Green's functions),

$$\begin{aligned}
F_N^{(1)} = & -\frac{i}{\hbar} \frac{1}{2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \\
& \times [-i\hbar G_0(x_2, t_1; x_1, t_1^+) (i\hbar G_0(x_1, t_1; x_2, t_1^+) i\hbar G_0(x, t; x', t') - \\
& i\hbar G_0(x, t; x_2, t_1) i\hbar G_0(x_1, t_1; x', t')) \\
& + i\hbar G_0(x_1, t_1; x_1, t_1^+) (i\hbar G_0(x_2, t_1; x_2, t_1^+) i\hbar G_0(x, t; x', t') - \\
& i\hbar G_0(x, t; x_2, t_1) i\hbar G_0(x_2, t_1; x', t')) \\
& + i\hbar G_0(x, t; x_1, t_1) (i\hbar G_0(x_1, t_1; x_2, t_1^+) i\hbar G_0(x_2, t_1; x', t') - \\
& i\hbar G_0(x_2, t_1; x_2, t_1^+) i\hbar G_0(x_1, t_1; x', t'))] .
\end{aligned}$$

The same procedure can be applied for the denominator when $n = 1$. In this case, one has only two non-vanishing contraction products. These are the disconnected diagrams from the previous equation:

$$\begin{aligned}
F_D^{(1)} = & -\frac{i}{\hbar} \frac{1}{2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \\
& \times [-i\hbar G_0(x_2, t_1; x_1, t_1^+) i\hbar G_0(x_1, t_1; x_2, t_1^+) \\
& + i\hbar G_0(x_1, t_1; x_1, t_1^+) i\hbar G_0(x_2, t_1; x_2, t_1^+)] \quad (D.10)
\end{aligned}$$

The interpretation of the equations for the numerator and the denominator are given in Appendix E. Wick's theorem can be applied for all the other interaction effects between particles like carrier-phonon scattering or impurity-scattering and for higher-order perturbations, i.e. for $n = 1, 2, \dots, \infty$. This is straightforward but requires a lot of place and concentration due to the form of the equations. The Feynman diagrams described in Appendix E provide a better way to solve the many-body problems and illustrate the perturbation expansion of the Green's functions.

Appendix E

Feynman Diagrams

Feynman diagrams represent the different contributions obtained from the Wick's decomposition (Appendix D), but in a shorter way. Therefore, the Green's functions G can be represented by an infinite sum of Feynman diagrams, each term of the sum corresponding to a decomposition of G into contracted products. For example, the perturbation expansion of the first order given in equation (D.10) generates six diagrams, but not all are different. There are a lot of rules to handle with these diagrams, depending on the Green's functions (equilibrium, non-equilibrium, zero or finite temperature ...). They are well explained for example in [20], [5], [11] or [10]. Here, one will only show how to work with the Feynman diagrams when the rules are known and one will only briefly repeat the main features of the diagrams.

E.1 Definitions

The Green's function

$$G(xt; x't') = -\frac{i}{\hbar} \langle \hat{\psi}_H(x, t) \hat{\psi}^\dagger(x', t') \rangle \quad (\text{E.1})$$

can be interpreted as the creation of a particle at point (x', t') , the propagation of the corresponding perturbation to the point (x, t) , where the particle is annihilated. Hence, the full Green's functions are represented by a double line (no i for Matsubara Green's functions) joining these two points

$$(x', t') \begin{array}{c} \text{=====} \blacktriangleright \text{=====} \\ i\hbar G(xt; x't') \end{array} (x, t). \quad (\text{E.2})$$

The non-interacting Green's functions are characterized by a single line and are proportional to the contraction of a creation and an annihilation field-operator in

the interaction picture

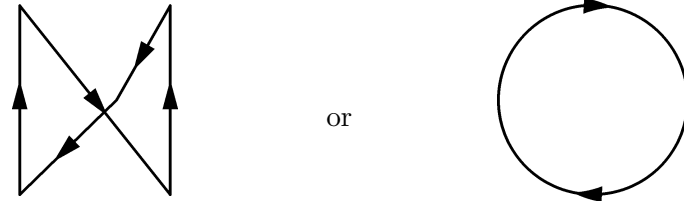
$$(x', t') \xrightarrow{i\hbar G_0(xt; x't')} (x, t). \quad (\text{E.3})$$

The Coulomb interaction $V(x_1 - x_2)$ becomes a wavy line with two inputs and two outputs which can be coupled together to describe a self-interaction (for example, an electron is knocked out of a state at time t and comes back to this state at this same time t , diagram for the Hartree potential)



$$-\frac{i}{\hbar} V(x_1 - x_2). \quad (\text{E.4})$$

Each time a Fermion loop occurs (i.e. it is possible to start from one point and to reach the same point again following only free Green's functions), the perturbation expression corresponding to this Feynman diagram must be multiplied by a factor (-1) . Example of Fermion loops



or

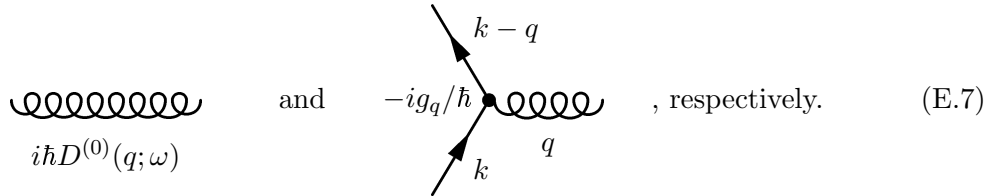
$$(\text{E.5})$$

The last important point for Fermion Green's functions concerns the internal variables available in nearly every Feynman diagram. They could be space x and time t or wave vector k and frequency ω , or a combination of them. Because these variables describe events taking place between the start and the end of the Green's function, but without any constraints for the exact time or place, they must be integrated or summed over the considered time, place, room, or frequency domain

$$(x', t') \xrightarrow{(x_1 t_1)} (x, t) \quad \Rightarrow \quad \int dt_1 \int dx_1. \quad (\text{E.6})$$

where x_1 and t_1 represent the time and the place at which the internal event symbolized by the black dot occurs.

The carriers can also interact with phonons: it is necessary to define the diagrams for these physical quantities. For phonons, it is better to work in the (k, ω) -space than in the (x, t) -space. A free phonon and the interaction between carriers and phonons are represented by



The diagram shows two Feynman symbols. On the left is a horizontal wavy line representing a free phonon, labeled below as $i\hbar D^{(0)}(q; \omega)$. To its right is the word "and". To the right of "and" is a vertex diagram: a wavy line (phonon) with momentum q enters from the right, and two straight lines (carriers) meet at a central dot. One carrier line enters from the bottom-left with momentum k , and the other exits to the top-right with momentum $k - q$. The vertex is labeled $-ig_q/\hbar$. To the right of this vertex diagram is the word " , respectively." followed by the equation number (E.7).

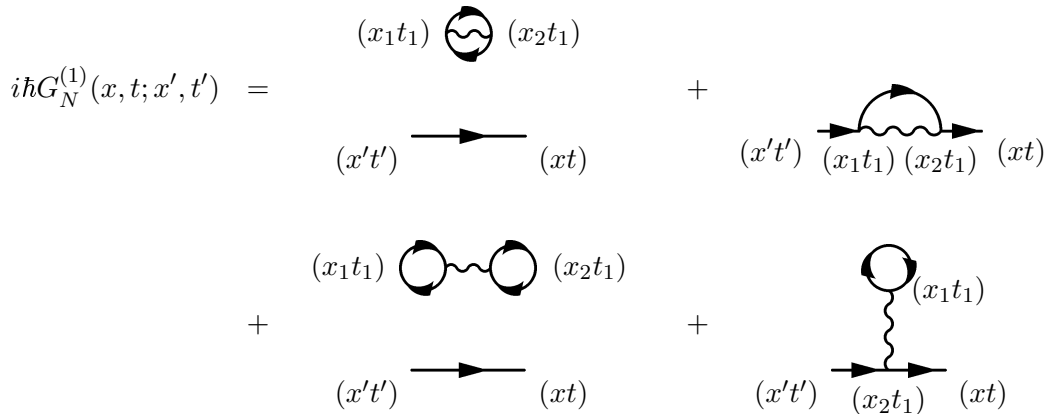
E.2 Simple Application

In this section, one will study the perturbation expansion of a Green's function resulting from the Wick's decomposition for the carrier-carrier interaction. Many orders of perturbation occur in the expansion

$$G(x, t; x', t') = G^{(0)}(x, t; x', t') + G^{(1)}(x, t; x', t') + G^{(2)}(x, t; x', t') + \dots \quad (\text{E.8})$$

For quantum transport, this hierarchy is usually stopped after the second order because this mini-series already contains the Hartree-Fock renormalization and the collision between carriers, the higher order terms being considered implicitly through screening, for example.

In equation (E.8), the first term $G^{(0)}(xt; x't')$ is obviously the free Green's function described by the Feynman diagram E.3. For the first order perturbation $G^{(1)}(xt; x't')$, one recalls equation (D.10) and transforms it into Feynman diagrams with the help of the rules formulated previously. The diagrams follow the same order as the terms in equation (D.10). First, only the numerator N is observed.



The equation shows the first-order perturbation expansion of the Green's function. On the left is the expression $i\hbar G_N^{(1)}(x, t; x', t') =$. This is followed by four Feynman diagrams separated by plus signs.
 1. The first diagram shows a horizontal straight line with arrows pointing right, representing a carrier. The left end is labeled $(x't')$ and the right end is labeled (xt) . Above this line is a wavy loop (phonon) with its left end labeled (x_1t_1) and its right end labeled (x_2t_1) .
 2. The second diagram shows a horizontal straight line with arrows pointing right, labeled $(x't')$ at the left and (xt) at the right. Above it is a wavy line (phonon) that starts at (x_1t_1) , goes up and right, then loops back down and left to (x_2t_1) .
 3. The third diagram shows a horizontal straight line with arrows pointing right, labeled $(x't')$ at the left and (xt) at the right. Above it are two wavy loops (phonons) connected in series. The first loop has ends (x_1t_1) and (x_2t_1) .
 4. The fourth diagram shows a horizontal straight line with arrows pointing right, labeled $(x't')$ at the left and (xt) at the right. Above it is a wavy line (phonon) that starts at (x_2t_1) , goes up and left, then loops back down and right to (x_1t_1) .

$$\begin{aligned}
& + \quad \text{Diagram 1: } (x't') \xrightarrow{(x_2t_1)} \text{loop} \xrightarrow{(x_1t_1)} (xt) \quad + \quad \text{Diagram 2: } (x't') \xrightarrow{(x_1t_1)} \text{loop} \xrightarrow{(x_2t_1)} (xt) \\
& \hspace{15em} \text{(E.9)}
\end{aligned}$$

For the denominator, only the first and the third diagram remain. They are called disconnected diagrams, because the interactions are not coupled to the line joining (x', t') and (x, t) . Two important consequences need to be highlighted:

- the disconnected diagrams from the denominator will cancel the disconnected diagrams from the numerator. This is due to the fact that higher-order terms in the perturbation, like $G_N^{(2)}(xt; x't')$ or $G_N^{(3)}(xt; x't')$ bring, among others, diagrams which are combination of connected and disconnected diagrams: in the second order perturbation, a Feynman diagram composed of the first and the second diagram of equation (E.9) is present

$$\begin{aligned}
& \text{Diagram 3: } (x_1t_1) \text{ loop } (x_2t_1) \\
& \text{Diagram 4: } (x't') \xrightarrow{(x_3t_3)} \text{loop} \xrightarrow{(x_4t_3)} (xt).
\end{aligned}$$

Considering all orders of perturbation, a common factor, the disconnected diagrams, can be extracted and is canceled by the denominator. Hence, it is only necessary to draw the connected Feynman diagrams to describe a Green's function.

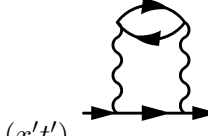
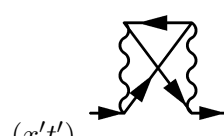
- in equation (D.10), the perturbation V is multiplied by a factor $\frac{1}{2}$, which disappears in the diagram expansion. The connected diagrams appear in pairs for the first order of perturbation (for example, the second and the fifth diagram) and it is obvious that they represent the same physical quantity. Only internal variables are exchanged and due to the integration of these variables (E.6), the two diagrams are equivalent. For each order n of the perturbation, the repetition of the same diagrams will compensate the factor $(\frac{1}{2})^n$ of the perturbation V^n and the factor $\frac{1}{n!}$ appearing in the development of the exponential function.

These two remarks hold for all orders of perturbation. As consequence, one has to draw only the different connected diagrams to compute the Green's function G . This gives for $G^{(1)}(x, t; x', t')$

$$i\hbar G^{(1)}(x, t; x', t') = \text{Diagram 5: } (x't') \xrightarrow{(x_1t_1)} \text{loop} \xrightarrow{(x_2t_1)} (xt) + \text{Diagram 6: } (xt) \xrightarrow{(x_1t_1)} \text{loop} \xrightarrow{(x_2t_1)} (x't').$$

Going through the second order perturbation $G^{(2)}(x, t; x', t')$, one obtains many different connected diagrams but the two most important are the direct and exchange collision contributions which occur eight times and therefore compensate the $\frac{1}{2!}$ and the $\frac{V_I}{2} \frac{V_I}{2}$ factors. This yields for these two terms

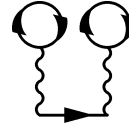
$$i\hbar G^{(2)}(x, t; x', t') = \text{diagram (a)} + \text{diagram (b)}.$$

(a)  (b) 

E.3 Equation of Motion and Self-Energy

Considering all the diagrams obtained by a perturbation expansion of the Green's function G , one sees that they all begin and end by a free Green's function G_0 . These two contributions can be treated separately and the middle part called *self-energy part* remains. Example of self-energy parts

$$\text{(a)} \quad \text{(b)} \quad \text{(c)} \quad \text{(d)} \quad \text{(e)} \quad (\text{E.10})$$

(a)  (b)  (c)  (d)  (e) 

There are two kinds of self-energy parts as it is obvious from equation (E.10)

- the *reducible* self-energy part. This is a self-energy part which can be divided into two other self-energy parts by removing a free Green's function G_0 like (a) and (d) in (E.10).
- the *proper* (or irreducible) self-energy part which can not be divided into two smaller self-energy parts by removing a free Green's function like (b), (c) and (e).

The sum of all proper self-energy parts coming from all the orders of perturbation is called *self-energy* and denoted by Σ . With the first order and the two most important diagrams of second order, one gets for the self-energy Σ

$$\begin{aligned} \textcircled{\Sigma} &= \text{diagram (b)} + \text{diagram (c)} + \text{diagram (a)} + \text{diagram (e)} + \dots \\ &= \left(-\frac{i}{\hbar}\right) \Sigma(x_1, t_1; x_2, t_2) \end{aligned} \quad (\text{E.11})$$

The proper self-energy parts contain only free Green's functions, but going to higher order perturbations and considering for example the second Feynman diagram in

equation (E.11), one notices the appearance of the following sum of parent diagrams

$$\begin{aligned}
 & \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \dots = \\
 & \text{Diagram 6} \times \left(\text{Diagram 7} + \text{Diagram 8} + \text{Diagram 9} + \text{Diagram 10} + \text{Diagram 11} + \dots \right) = \\
 & \text{Diagram 12} \times \left(\text{Diagram 13} \right) = \text{Diagram 14} \quad (\text{E.12})
 \end{aligned}$$

This means that every free Green's function in equation (E.11) must be replaced by a normal Green's function G , represented by a double line as in (E.2). This gives for the self-energy Σ the following self-consistent equation

$$\text{Diagram 15} = \text{Diagram 16} + \text{Diagram 17} + \text{Diagram 18} + \text{Diagram 19} + \dots$$

Then, the total Green's function $G(x, t; x', t')$ is nothing else than the sum of all the connected self-energy parts. Therefore, one can write all the Green's functions as

$$\begin{aligned}
 i\hbar G(x, t; x', t') &= \text{Diagram 20} + \text{Diagram 21} + \left(\text{Diagram 22} \right)^2 + \left(\text{Diagram 23} \right)^3 + \dots \\
 &= \text{Diagram 24} + \text{Diagram 25}
 \end{aligned}$$

Converting the Feynman diagrams into mathematical expressions yields


$$\begin{aligned}
 G(11') &= G_0(11') + \int d2 \int d3 G_0(12) \Sigma(23) G(31') \\
 \text{or} \\
 &= G_0(11') + \int d2 \int d3 G(12) \Sigma(23) G_0(31') \quad (\text{E.13})
 \end{aligned}$$

with $1 = (x, t)$ and $\int 1 = \int dx \int dt$. This is the equation of motion for the Green's function $G(11')$.

E.4 Screening

Repeating the same procedure as in equation (E.12) but extracting the interaction V instead of the free Green's function, one obtains the shielded interaction V_s or W . The only condition is that the considered Feynman diagrams must begin and end by an interaction V . This gives

$$\begin{aligned}
 -\frac{i}{\hbar}W(12) &= \text{wavy line} = \text{wavy line} + \text{bubble} + \text{two bubbles} + \text{three bubbles} \\
 &+ \text{four bubbles} + \text{bubble with a loop} + \text{bubble with two loops} + \dots
 \end{aligned}$$

Keeping only the Feynman diagrams which are combinations of the bubble diagram  preceded and followed by the interaction \sim , one gets the screened interaction within the *RPA* (Random Phase Approximation)

$$\begin{aligned}
 -\frac{i}{\hbar}W_{RPA}(12) &= \text{wavy line}_{RPA} = \text{wavy line} + \text{bubble} + \text{two bubbles} + \text{three bubbles} + \dots \\
 &= \text{wavy line} + \text{bubble}
 \end{aligned}$$

Converting the Feynman diagrams into mathematical expressions gives the following equation for the screened interaction within RPA


$$\begin{aligned}
 W_{RPA}(12) &= V(1-2) - i\hbar \int d3 \int d4 V(1-3)G(34)G(43)W_{RPA}(42) \\
 &= V(1-2) + \int d3 \int d4 V(1-3)\pi(34)W_{RPA}(42)
 \end{aligned} \tag{E.14}$$

with

$$V(1-2) = V(|x_1 - x_2|)\delta(t_1 t_2) \quad (\text{E.15})$$

and

$$\pi(12) = -i\hbar G(12)G(21) \quad (\text{E.16})$$

As consequence, one obtains a direct relation between the bubble diagram  and the factor $\pi(12)$ in the RPA approximation.

$$i\hbar\pi(12) = \text{bubble diagram} \quad (\text{E.17})$$

Special care must be taken to include the screened potential $W(12)$ into equation (E.11) for the self-energy Σ . The second diagram (Fock term) and the third (direct collision) require the same sum of diagrams to screen their interaction V . It is therefore impossible to have both terms screened at the same time and in most of the applications, the Fock term remains unscreened while W replaces V for the direct collision term.

As conclusion, the self-energies for the four different diagrams of equation (E.11) are given, including the total Green's function G instead of the free Green's function G_0 and the screened interaction W instead of V , if it is possible. One begins with the Hartree term (no screening because the sum required to replace V by W is not physical in this case)

$$\text{Hartree diagram} \Rightarrow \Sigma(12) = -i\hbar\delta(12) \int d3 V(1-3)G(33). \quad (\text{E.18})$$

The second first-order contribution is the Fock term where screening is not possible, because the sum of diagrams required for this effect is the same as for the direct collision contribution where screening will be used

$$\text{Fock diagram} \Rightarrow \Sigma(12) = i\hbar V(1-2)G(x_1, t_1; x_2, t_1). \quad (\text{E.19})$$

The direct collision term has only one interaction screened and not both, because the sum of diagrams required to screen the first interaction is the same as the sum required to screen the second interaction. Therefore, only one interaction V becomes W and one obtains

The replacement of V by the sum of the carrier-carrier and carrier-phonon interaction (zigzag line) is not possible for the Hartree term (first diagram).

The new screened interaction W_{eff} taking into account both the carrier-carrier and carrier-phonon interaction is given in the RPA approximation by the dressed zigzag line and the following equation:

$$-\frac{i}{\hbar}W_{eff}(12) = \text{zigzag} = \text{zigzag} + \text{loop with two zigzags}$$

For many applications, it is interesting to separate W_{eff} into two contributions, one resulting only from the screened carrier-carrier interaction W given in equation (E.14) and another from the carrier-phonon W^{ph} , including the influence of W . Hence, one has

$$-\frac{i}{\hbar}W^{ph}(12) = -\frac{i}{\hbar}(W_{eff} - W)(12) = \left(\text{zigzag} + \text{loop with two zigzags} \right) - \left(\text{wavy} + \text{loop with wavy and zigzag} \right)$$

To solve this diagram equation, the transformation into the (k, ω) space provides great advantages, because the equation for $W^{ph}(12)$ can be simplified. Fourier transforming space and time gives

$$\begin{aligned} -\frac{i}{\hbar}W^{ph}(k\omega) &= \frac{\text{zigzag}}{1 - \text{loop with zigzag}} - \frac{\text{wavy}}{1 - \text{loop with wavy}} \\ &= \frac{(\text{wavy} + \text{loop with wavy and zigzag})(1 - \text{loop with wavy}) - \text{wavy}(1 - \text{loop with wavy} - \text{loop with wavy and zigzag})}{(1 - \text{loop with zigzag})(1 - \text{loop with wavy})} \\ &= \frac{\text{loop with wavy and zigzag}}{(1 - \text{loop with zigzag})(1 - \text{loop with wavy})} = \frac{\text{loop with wavy and zigzag}}{(1 - \text{loop with wavy} - \text{loop with wavy and zigzag})(1 - \text{loop with wavy})} \\ &= \frac{\text{loop with wavy and zigzag}}{\left(1 - \frac{\text{loop with wavy and zigzag}}{1 - \text{loop with wavy}}\right)(1 - \text{loop with wavy})^2} = \text{zigzag with many loops} \end{aligned}$$

(E.22)

where the last diagram of equation (E.22) represents the dressed phonon interaction. This interaction contains different parameters:

- the intraband susceptibility $\chi(k, \omega)$ which obeys the following equation

$$i\hbar\chi(k, \omega) = \text{diagram} = \frac{\text{diagram}}{1 - \text{diagram}} = \text{diagram} + \text{diagram}$$

The diagram on the left is a loop with a wavy line and a label χ . The denominator diagram is a loop with a wavy line. The first term on the right is a loop with a straight line. The second term on the right is a loop with a wavy line and a label χ .

- the phonon dressed line governed by this equation:

$$i\hbar D(k, \omega) = \text{diagram} = \frac{\text{diagram}}{1 - \text{diagram}} = \text{diagram} + \text{diagram}$$

The diagram on the left is a wavy line with a label D . The denominator diagram is a loop with a wavy line and a label χ . The first term on the right is a wavy line. The second term on the right is a loop with a wavy line and a label χ .

- and the dressed interaction given by:

$$-\frac{i}{\hbar}g_q^{eff} = \text{diagram} = \frac{\text{diagram}}{1 - \text{diagram}}$$

The diagram on the left is a circle with a dot in the center. The denominator diagram is a loop with a wavy line.

Fourier-transforming back in the time domain, but remaining in the k -space yields following equations for the intraband susceptibility $\chi(q; t_1 t_2)$, the phonon Green's function $D(q; t_1 t_2)$ and the dressed electron-phonon interaction $W^{ph}(q; t_1 t_2)$:

$$\chi(q; t_1 t_2) = \pi(q; t_1 t_2) + \int dt_3 V_q \pi(q; t_1 t_3) \chi(q; t_3 t_2)$$

$$D(q; t_1 t_2) = D^{(0)}(q; t_1 t_2) + \int dt_3 \int dt_4 g_q^2 D^{(0)}(q; t_1 t_3) \chi(q; t_3 t_4) D(q; t_4 t_2)$$

$$W^{ph}(q; t_1 t_2) = \int dt_3 \int dt_4 g_q^2 \epsilon^{-1}(q; t_1 t_3) D(q; t_3 t_4) \epsilon^{-1}(q; t_4 t_2)$$

Appendix F

Self-Energy Variational Derivation

The equations of motion (2.2) and (2.3) for $G(11')$ depend on the two-particle Green's function $G^{(2)}(1323)$ defined in equation (2.4). To evaluate $G^{(2)}(1323)$, there are two possibilities:

- either to write a new equation of motion for it, which will be coupled with a three-particle Green's function $G^{(3)}$, in turn coupled with a four-particle Green's function $G^{(4)}$, leading to infinite hierarchy
- or to try to express it as products of single particle Green's functions $G(11')$, yielding an infinite perturbation expansion. This is the more convenient method [2, 11, 9, 13].

To derive this perturbation theory, one has to study how a nonequilibrium Green's function $G(11')$ reacts after the changes of the external potential $U(x, t)$ applied on the system: hence, the central point is the quantity $\frac{dG(11')}{dU(3)}$. Recalling equations (1.45) and (1.46), one obtains

$$\begin{aligned}
\frac{dG(11')}{dU(3)} &= -\frac{i}{\hbar} \frac{\langle T \left\{ \frac{dS_H^{ext}(t_0, t_0)}{dU(3)} \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\
&\quad - \frac{i}{\hbar} \frac{\langle T \left\{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \cdot \frac{\langle -\frac{dS_H^{ext}(t_0, t_0)}{dU(3)} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\
&= -\left(-\frac{i}{\hbar}\right)^2 \frac{\langle T \left\{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(1) \hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) \hat{\psi}_H^\dagger(1') \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\
&\quad + G(11') \cdot \left(-\frac{i}{\hbar}\right) \frac{\langle T \left\{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\
&= -G(13^- 1' 3^+) + G(11') G(33^+). \tag{F.1}
\end{aligned}$$

Inserting this final result into equation (2.2) yields

$$\begin{aligned}
 \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1) \right) G(11') &= \delta(11') + i\hbar \int_C d3 V(1-3) \frac{dG(11')}{dU(3)} \\
 &\quad - i\hbar \int_C d3 V(1-3) G(33^+) G(11') \\
 &= \delta(11') + \int_C d2 \Sigma^{tot}(12) G(21')
 \end{aligned} \tag{F.2}$$

where the total self-energy $\Sigma^{tot}(12) = \Sigma_{Hartree}(12) + \Sigma(12)$. First, the Hartree self-energy $\Sigma_{Hartree}(12)$ will be considered. If one compares the first and the second line of equation (F.2), one finds that

$$\Sigma_{Hartree}(12) = -i\hbar \delta(12) \int_C d3 V(1-3) G(33^+) \tag{F.3}$$

in accordance with the result previously obtained with the Feynman diagrams in equation (E.18). It is more complicated to derive an expression for $\Sigma(12)$ from equation (F.2). For that purpose, one needs to define the inverse Green's function $G^{-1}(12)$ with the following property on contour C from figure 1.1

$$\int_C d2 G^{-1}(12) G(21') = \int_C d2 G(12) G^{-1}(21') = \delta(11') \tag{F.4}$$

which only holds, if the conditions required by the Wick's decomposition in Appendix D are fulfilled by the Green's function $G(12)$ on contour C . If, for example, initial correlations are present at t_0 , then the contour of figure 1.1 must be deformed to take them into account. This point will be explained in Appendix H. Recalling equation (F.2) and the property of the inverse Green's function $G^{-1}(12)$ yields

$$\begin{aligned}
 i\hbar \int_C d3 V(1-3) \frac{dG(11')}{dU(3)} &= i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(14)}{dU(3)} \delta(41') \\
 &= i\hbar \int_C d2 \int_C d3 \int_C d4 V(1-3) \frac{dG(14)}{dU(3)} G^{-1}(42) G(21') \\
 &= \int_C d2 \int_C \Sigma(12) G(21')
 \end{aligned} \tag{F.5}$$

and

$$\Sigma(12) = i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(14)}{dU(3)} G^{-1}(42). \tag{F.6}$$

To define the self-energy $\Sigma(12)$, which contains information on the renormalization of the one-particle energies as well as the scattering rates, and to derive its perturbation expansion, only the existence of the inverse Green's function $G^{-1}(12)$ on

the contour C is required, but not its explicit form. Technically, the perturbation expansion is based on a repeated change of variables in equation (F.6). First, one introduces the additional functions generated by the change of variables:

- the longitudinal polarization function $\pi(12)$, already defined via the Feynman diagrams in equation (E.16), which describes the possible one-particle transitions as a result of longitudinal electric fields,
- the screened Coulomb potential $W(12)$, introduced in section E.4, which differs from the bare Coulomb potential $V(1-2)$ because of one-particle transition possibilities as described by $\pi(12)$,
- the vertex function $\Gamma(123)$ to complete formally the set of equations.

To take account of the screening effects, one has to define an effective perturbation $U_{eff}(1)$, containing both $U(1)$ and the Hartree self-energy $\Sigma_{Hartree}(12)$, with

$$U_{eff}(1) = U(1) - i\hbar \int_C d2 V(1-2)G(22^+). \quad (F.7)$$

One starts from equation (F.6) and repeatedly changes variables:

$$\begin{aligned} \Sigma(12) &= i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(14)}{dU(3)} G^{-1}(42) \\ &= -i\hbar \int_C d3 \int_C d4 V(1-3) G(14) \frac{dG^{-1}(42)}{dU(3)} \\ &= -i\hbar \int_C d3 \int_C d4 \int_C d5 V(1-3) G(14) \frac{dG^{-1}(42)}{dU_{eff}(5)} \frac{dU_{eff}(5)}{dU(3)} \\ &= -i\hbar \int_C d4 \int_C d5 W(51) G(14) \Gamma(425). \end{aligned} \quad (F.8)$$

The transition from the first line to the second was obtained because

$$\begin{aligned} \frac{d}{dU(3)} \left[\int_C d2 G(12) G^{-1}(21') \right] &= \frac{d\delta(11')}{dU(3)} = 0 \\ &= \int_C d2 \frac{dG(12)}{dU(3)} G^{-1}(21') + \\ &\quad \int_C d2 G(12) \frac{dG^{-1}(21')}{dU(3)}. \end{aligned} \quad (F.9)$$

In going from the third to the fourth line, one introduced the screened Coulomb potential

$$W(21) = \int_C d3 V(1-3) \frac{dU_{eff}(2)}{dU(3)} \quad (F.10)$$

and the vertex function

$$\Gamma(123) = \frac{dG^{-1}(12)}{dU_{eff}(3)}. \quad (F.11)$$

Recalling the definition of $U_{eff}(1)$ from equation (F.7) and inserting it into (F.10) yields

$$\begin{aligned} \frac{dU_{eff}(1)}{dU(2)} &= \delta(12) - i\hbar \int_C d3 V(1-3) \frac{dG(33^+)}{dU(2)} \\ &= \delta(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}(4)} \frac{dU_{eff}(4)}{dU(2)} \end{aligned} \quad (F.12)$$

and

$$\begin{aligned} W(21) &= V(1-2) - i\hbar \int_C d3 \int_C d4 \int_C d5 V(1-3)V(2-4) \frac{dG(44^+)}{dU_{eff}(5)} \frac{dU_{eff}(5)}{dU(3)} \\ &= V(1-2) - i\hbar \int_C d4 \int_C d5 V(2-4) \frac{dG(44^+)}{dU_{eff}(5)} W(51) \\ &= V(1-2) + \int_C d4 \int_C d5 V(2-4) \pi(45) W(51), \end{aligned} \quad (F.13)$$

where the polarization function is defined in the following way

$$\begin{aligned} \pi(12) &= -i\hbar \frac{dG(11^+)}{dU_{eff}(2)} \\ &= -i\hbar \int_C d3 \int_C d4 \frac{dG(13)}{dU_{eff}(2)} G^{-1}(34) G(41^+) \\ &= i\hbar \int_C d3 \int_C d4 G(13) \frac{dG^{-1}(34)}{dU_{eff}(2)} G(41^+) \\ &= i\hbar \int_C d3 \int_C d4 G(13) \Gamma(342) G(41^+). \end{aligned} \quad (F.14)$$

It remains to make changes of variables for the vertex function. For that purpose, an expression for $G^{-1}(12)$ is required, which is obtained from the slightly modified equation of motion (2.5)

$$\begin{aligned} \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U_{eff}(1) \right) G(12) &= \int_C d3 \left[G_{eff}^{(0)}(13) \right]^{-1} G(32) \\ &= \delta(12) + \int_C d3 \Sigma(13) G(32) \end{aligned} \quad (F.15)$$

with

$$\left[G_{eff}^{(0)}(12) \right]^{-1} = \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U_{eff}(1) \right) \delta(12). \quad (F.16)$$

Multiplying and integrating each line of equation (F.15) by $\int_C d2 G^{-1}(21')$, one finds that

$$\left[G_{eff}^{(0)}(11') \right]^{-1} = G^{-1}(11') + \Sigma(11') \quad (F.17)$$

or

$$G^{-1}(11') = \left[G_{eff}^{(0)}(11') \right]^{-1} - \Sigma(11'). \quad (\text{F.18})$$

The vertex function Γ is now defined by

$$\begin{aligned} \Gamma(123) &= \frac{dG^{-1}(12)}{dU_{eff}(3)} \\ &= \frac{d \left[G_{eff}^{(0)}(12) \right]^{-1}}{dU_{eff}(3)} - \frac{d\Sigma(12)}{dU_{eff}(3)} \\ &= -\delta(12)\delta(13) - \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG(45)} \frac{dG(45)}{dU_{eff}(3)} \\ &= -\delta(12)\delta(13) \\ &\quad - \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG(45)} \int_C d6 \int_C d7 \frac{dG(46)}{dU_{eff}(3)} G^{-1}(67)G(75) \\ &= -\delta(12)\delta(13) \\ &\quad + \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG(45)} \int_C d6 \int_C d7 G(46) \frac{dG^{-1}(67)}{dU_{eff}(3)} G(75) \\ &= -\delta(12)\delta(13) \\ &\quad + \int_C d4 \int_C d5 \int_C d6 \int_C d7 \frac{d\Sigma(12)}{dG(45)} G(46)\Gamma(673)G(75). \end{aligned} \quad (\text{F.19})$$

This is the starting point of the perturbation theory. The equation for the vertex function Γ is reiterated and each time inserted in the equations for the polarization function π , the screened Coulomb potential W and the self-energy Σ , which in turn contributes to the next iteration of Γ :

$$\begin{aligned} \Gamma &= \Gamma^{(0)} + \Gamma^{(1)}(\Sigma^{(0)}, \Gamma^{(0)}) + \Gamma^{(2)}(\Sigma^{(1)}, \Gamma^{(1)}, \Sigma^{(0)}, \Gamma^{(0)}) + \dots \\ \pi &= \pi^{(0)}(\Gamma^{(0)}) + \pi^{(1)}(\Gamma^{(1)}) + \pi^{(2)}(\Gamma^{(2)}) + \dots \\ W &= W^{(0)}(\pi^{(0)}) + W^{(1)}(\pi^{(1)}) + W^{(2)}(\pi^{(2)}) + \dots \\ \Sigma &= \Sigma^{(00)}(W^{(0)}, \Gamma^{(0)}) + \Sigma^{(10)}(W^{(1)}, \Gamma^{(0)}) + \Sigma^{(01)}(W^{(0)}, \Gamma^{(1)}) + \dots \end{aligned} \quad (\text{F.20})$$

where the first iteration is $\Gamma^{(0)}(123) = -\delta(12)\delta(13)$, according to equation (F.19).

F.1 First Iteration

In the first iteration, the polarization function π is replaced by

$$\begin{aligned} \pi(12) &= \pi^{(0)}(12) \\ &= i\hbar \int_C d3 \int_C d4 G(13)\Gamma^{(0)}(342)G(41^+) \\ &= -i\hbar G(12)G(21^+) \end{aligned} \quad (\text{F.21})$$

and then inserted into the equation for the screened Coulomb potential (F.13), which becomes $W_{RPA} = W^{(0)}$ instead of W . This approximation for the screened potential is called RPA for Random Phase Approximation and one obtains for the self-energy

$$\begin{aligned}
\Sigma(12) &= \Sigma^{(0)}(12) \\
&= -i\hbar \int_C d4 \int_C d5 W^{(0)}(51)G(14)\Gamma^{(0)}(425) \\
&= i\hbar \int_C d4 \int_C d5 W_{RPA}(51)G(14)\delta(42)\delta(45) \\
&= i\hbar W_{RPA}(21)G(12).
\end{aligned} \tag{F.22}$$

For the later treatment of the time dependence of the self-energy Σ , it is convenient to separate it into two parts resulting from equation (F.13) for the screened potential

$$\begin{aligned}
\Sigma(12) &= i\hbar W_{RPA}(21)G(12) \\
&= i\hbar V(1-2)G(12) + i\hbar \int_C d4 \int_C d5 V(2-4)\pi(45)W_{RPA}(51)G(12).
\end{aligned} \tag{F.23}$$

F.1.1 Fock Self-Energy

The first part of equation (F.23) is instantaneous because $V(1-2) = V(x_1 - x_2)\delta(t_1 t_2)$ and is called Fock self-energy, defined by

$$\Sigma_{Fock}(12) = i\hbar V(1-2)G(12) \tag{F.24}$$

and in accordance with equation (E.19) resulting from the Feynman diagrams. It can be combined with the previously defined Hartree self-energy to form an instantaneous part of the total self energy [11]

$$\Sigma^{tot}(12) = \Sigma^\delta(12) + \Sigma(12) \tag{F.25}$$

with

$$\begin{aligned}
\Sigma^\delta &= \Sigma_{Hartree} + \Sigma_{Fock} \\
&= i\hbar V(1-2)G(12) - i\hbar \delta(12) \int_C d3 V(1-3)G(33^+).
\end{aligned} \tag{F.26}$$

F.1.2 Direct Collision Self-Energy

The second part of equation (F.23) is the direct collision self-energy given by

$$\Sigma_{dc}(12) = i\hbar \int_C d3 \int_C d4 V(2-3)\pi(34)W(41)G(12). \tag{F.27}$$

This result is similar to the Feynman diagram equation (E.20).

F.2 Vertex Correction

To get the next order of perturbation for the self-energy, while keeping the RPA for the screened Coulomb potential, one has to consider Σ^{01} where the vertex function $\Gamma^{(1)}(123)$ occurs.

$$\begin{aligned}\Gamma^{(1)}(123) &= \int_C d4 \int_C d5 \int_C d6 \int_C d7 \frac{d\Sigma^{(0)}(12)}{dG(45)} G(46) \Gamma^{(0)}(673) G(75) \\ &= - \int_C d4 \int_C d5 \frac{d\Sigma^{(0)}(12)}{dG(45)} G(43) G(35)\end{aligned}\quad (\text{F.28})$$

where

$$\begin{aligned}\frac{d\Sigma^{(0)}(12)}{dG(45)} &= i\hbar W(21) \frac{dG(12)}{dG(45)} \\ &= i\hbar W(21) \delta(14) \delta(25).\end{aligned}\quad (\text{F.29})$$

Therefore $\Gamma^{(1)}$ becomes

$$\Gamma^{(1)}(123) = -i\hbar W(21) G(13) G(32). \quad (\text{F.30})$$

This gives for the self-energy $\Sigma_{ex}(12) = \Sigma^{(01)}(12)$, which describes the exchange collision effects:

$$\begin{aligned}\Sigma_{ex}(12) &= -i\hbar \int_C d3 \int_C d4 W(31) G(14) \Gamma^{(1)}(423) \\ &= -(\hbar)^2 \int_C d3 \int_C d4 W(31) G(14) G(43) G(32) W(42)\end{aligned}\quad (\text{F.31})$$

in accordance to Feynman diagram from equation (E.21).

F.3 Carrier-Phonon Interaction

The influence of the nuclei on the carriers (carrier-phonon interaction) can be taken into account by considering the following potential

$$V^{c-n} = \int d2 V(1-2) \rho^n(2), \quad (\text{F.32})$$

where $V(1-2)$ is the Coulomb potential between a particle at position x_1 and $\rho^n(2)$, the nuclei density, at position x_2 . This gives in the second quantization

$$\begin{aligned}H^{c-n} &= \int d1 \int d2 V(1-2) \hat{\psi}^\dagger(1) \hat{\psi}(1) \rho^n(2) \\ &= \int d1 \int d2 V(1-2) \rho^{el}(1) \rho^n(2).\end{aligned}\quad (\text{F.33})$$

Then the total Hamiltonian $\mathcal{H}(t)$ contains the unperturbed part H^0 , the carrier-carrier interaction V , the carrier-nuclei interaction H^{c-n} and an external perturbation $H^{ext}(t)$ acting both on the carriers and the nuclei

$$H^{ext}(t) = \int dx U(x, t) \left(\rho^{el}(x, t) + \rho^n(x, t) \right). \quad (\text{F.34})$$

The equation of motion for the Green's function $G(11')$ given by equation (1.46) but including the carrier-nuclei interaction has the following form

$$\begin{aligned} \left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1) - \int_C d3 V(1-3) \langle \rho^n(3) \rangle \right) G(11') = \\ \delta(11') - i\hbar \int_C d3 V(1-3) G^{(2)}(13^+ 23^{++}). \end{aligned} \quad (\text{F.35})$$

This is done with

$$\begin{aligned} i\hbar T \left\{ \frac{d}{dt} \left(S_H^{ext}(t_0, t_0) \hat{\psi}_H(x, t) \right) \right\} &= T \left\{ i\hbar \frac{d}{dt} \left(S_H^{ext}(t_0, t) \hat{\psi}_H(x, t) S_H^{ext}(t, t_0) \right) \right\} \\ &= T \left\{ S_H^{ext}(t_0, t_0) i\hbar \frac{d}{dt} \hat{\psi}_H(x, t) \right\} \\ &+ i\hbar T \left\{ S_H^{ext}(t_0, t_0) \int dx_2 U(x_2, t) \left[\hat{\psi}_H(1), \rho^{el}(x_2) + \rho^n(x_2) \right] \right\} \\ &= T \left\{ S_H^{ext}(t_0, t_0) i\hbar \frac{d}{dt} \hat{\psi}_H(x, t) \right\} + i\hbar T \left\{ S_H^{ext}(t_0, t_0) U(1) \hat{\psi}_H(1) \right\} \end{aligned}$$

and

$$\begin{aligned} i\hbar \frac{d}{dt} \hat{\psi}_H(x, t) &= \left[\hat{\psi}_H(x, t), H_H(t) \right] \\ &= -\frac{\hbar^2 \nabla_x^2}{2m} \hat{\psi}_H(x, t) + \int dy V(x-y) \hat{\psi}_H^\dagger(y, t) \hat{\psi}_H(y, t) \hat{\psi}_H(x, t) \\ &+ \int dy V(x-y) \rho^n(y, t) \hat{\psi}_H(x, t). \end{aligned}$$

Furthermore, modifying equation (F.1) to take into account the carrier-phonon interaction yields

$$\begin{aligned} \frac{dG(11')}{dU(3)} &= - \left(-\frac{i}{\hbar} \right)^2 \frac{\langle T \left\{ S_H^{ext}(t_0, t_0) \hat{\psi}_H(1) \left(\hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) + \rho^n(3) \right) \hat{\psi}_H^\dagger(1') \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\ &+ G(11') \cdot \left(-\frac{i}{\hbar} \right) \frac{\langle T \left\{ S_H^{ext}(t_0, t_0) \left(\hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) + \rho^n(3) \right) \right\} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle} \\ &= -G(13^+ 1' 3^{++}) - G(11') A(3) + G(11') (G(33^+) + A(3)) \\ &= -G(13^+ 1' 3^{++}) + G(11') G(33^+), \end{aligned} \quad (\text{F.36})$$

where

$$A(3) = -\frac{i}{\hbar} \frac{\langle T \{ S_H^{ext}(t_0, t_0) \rho^n(3) \} \rangle}{\langle S_H^{ext}(t_0, t_0) \rangle}.$$

Using equation (F.36) and the equality $\langle \rho^{el}(1) \rangle = -i\hbar G(11^+)$ allows to rewrite equation (F.35) as

$$\left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1) - \int_C d3 V(1-3) \left(\langle \rho^{el}(3) \rangle + \langle \rho^n(3) \rangle \right) \right) G(11') = \delta(11') + i\hbar \int_C d3 V(1-3) \frac{dG(11')}{dU(3)}.$$

Therefore, with the same procedure as at the beginning of this Appendix, one obtains for the effective external potential

$$\begin{aligned} U_{eff}(1) &= U(1) - i\hbar \int_C d2 V(1-2) G(22^+) + \int_C d2 V(1-2) \langle \rho^n(2) \rangle \\ &= U(1) + \int_C d2 V(1-2) \left(\langle \rho^{el}(2) \rangle + \langle \rho^n(2) \rangle \right) \end{aligned} \quad (F.37)$$

which implies

$$\left(i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U_{eff}(1) \right) G(11') = \delta(11') + i\hbar \int_C d3 V(1-3) \frac{dG(11')}{dU(3)}. \quad (F.38)$$

In order to compute the carrier-phonon interaction, one has to introduce a source term in the external Hamiltonian $H^{ext}(t)$ from equation (F.34) [13]

$$H^{ext}(t) = \int dx \left[U(x, t) \left(\rho^{el}(x, t) + \rho^n(x, t) \right) + J(x, t) \rho^n(x, t) \right]. \quad (F.39)$$

The importance of this source term becomes clear in the variational derivation of the interaction. Starting from equation (F.12) yields for the derivative of the effective potential

$$\begin{aligned} \frac{dU_{eff}(1)}{dU(2)} &= \delta(12) + \int_C d3 V(1-3) \left(\frac{d\langle \rho^{el}(3) \rangle}{dU(2)} + \frac{d\langle \rho^n(3) \rangle}{dU(2)} \right) \\ &= \delta(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}(4)} \frac{dU_{eff}(4)}{dU(2)} \\ &\quad + \int_C d3 V(1-3) \frac{d\langle \rho^n(3) \rangle}{dU(2)}. \end{aligned} \quad (F.40)$$

One can rewrite this equation

$$\int_C d4 K(14) \frac{dU_{eff}(4)}{dU(2)} = \delta(12) + \int_C d3 V(1-3) \frac{d\langle \rho^n(3) \rangle}{dU(2)} \quad (F.41)$$

with

$$K(12) = \delta(12) + i\hbar \int_C d3 V(1-3) \frac{dG(33^+)}{dU_{eff}(2)} \quad (F.42)$$

Afterward, one defines the inverse dielectric function $\epsilon^{-1}(12)$ without the influence of carrier-phonon interaction by the following equation similar to (F.12)

$$\begin{aligned} \epsilon^{-1}(12) &= \frac{dU_{eff}^{el}(1)}{dU(2)} \\ &= \delta(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}^{el}(4)} \epsilon^{-1}(42), \end{aligned} \quad (F.43)$$

where U_{eff}^{el} contains only the influence of carrier-carrier scattering. Assuming that for weak carrier-phonon interaction $U_{eff} \simeq U_{eff}^{el}$, one finds

$$K(12) = \epsilon(12) \quad (F.44)$$

because of equation (F.43) and

$$\begin{aligned} \int_C d4 K(14) \epsilon^{-1}(42) &= \epsilon^{-1}(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}(4)} \epsilon^{-1}(42) \\ &\simeq \delta(12). \end{aligned} \quad (F.45)$$

The consequence for equation (F.41) is

$$\begin{aligned} \frac{dU_{eff}(4)}{dU(2)} &= \epsilon^{-1}(12) + \int_C d3 \int_C d4 \epsilon^{-1}(13) V(3-4) \frac{d\langle \rho^n(4) \rangle}{dU(2)} \\ &= \epsilon^{-1}(12) + \int_C d3 W(13) \frac{d\langle \rho^n(3) \rangle}{dU(2)}. \end{aligned} \quad (F.46)$$

It remains to evaluate the derivative of the nuclei density $\frac{d\langle \rho^n(3) \rangle}{dU(2)}$. For that purpose, one introduces the expectation value of the nuclei similar to the Green's function for electrons and holes

$$\langle \rho^n(1) \rangle = \frac{\langle T\{S\rho^n(1)\} \rangle}{\langle S \rangle}. \quad (F.47)$$

This enables to calculate the reaction of the nuclei under the action of the external potential $U(x, t)$

$$\begin{aligned} \frac{d\langle \rho^n(1) \rangle}{dU(2)} &= -\frac{i}{\hbar} \frac{\langle T\{S[\rho^{el}(2) + \rho^n(2)] \rho^n(1)\} \rangle}{\langle S \rangle} \\ &+ \frac{i}{\hbar} \frac{\langle T\{S\rho^n(1)\} \rangle \langle T\{S[\rho^{el}(2) + \rho^n(2)]\} \rangle^2}{\langle S \rangle} \\ &= -\frac{i}{\hbar} \frac{\langle T\{S[\Delta\rho^{el}(2) + \Delta\rho^n(2)] \Delta\rho^n(1)\} \rangle}{\langle S \rangle}, \end{aligned} \quad (F.48)$$

where $\Delta\rho = \rho - \langle\rho\rangle$. Equation (F.48) results from the fact that $\langle XY \rangle - \langle X \rangle \langle Y \rangle = \langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle$. The source term in $H^{ext}(t)$ plays an important role to evaluate (F.48). First, one considers the reaction of $\langle\rho^n\rangle$ and $\langle\rho^{el}\rangle$ on a variation of the source

$$\begin{aligned} \frac{d\langle\rho^n(1)\rangle}{dJ(2)} &= -\frac{i}{\hbar} \frac{\langle T\{S\Delta\rho^n(2)\Delta\rho^n(1)\}\rangle}{\langle S \rangle} \\ &= \mathcal{D}(12) \end{aligned} \quad (\text{F.49})$$

and

$$\frac{d\langle\rho^{el}(1)\rangle}{dJ(2)} = -\frac{i}{\hbar} \frac{\langle T\{S\Delta\rho^n(2)\Delta\rho^{el}(1)\}\rangle}{\langle S \rangle}. \quad (\text{F.50})$$

Going back to equation (F.48), one finds

$$\begin{aligned} \frac{d\langle\rho^n(1)\rangle}{dU(2)} &= \frac{d\langle\rho^n(2)\rangle}{dJ(1)} + \frac{d\langle\rho^{el}(2)\rangle}{dJ(1)} \\ &= \mathcal{D}(12) + \int_C d3 \frac{d\langle\rho^{el}(2)\rangle}{dU_{eff}(3)} \frac{dU_{eff}(3)}{dJ(1)} \\ &= \mathcal{D}(12) + \int_C d3 \int_C d4 \frac{d\langle\rho^{el}(2)\rangle}{dU_{eff}(3)} V(3-4) \left(\frac{d\langle\rho^{el}(4)\rangle}{dJ(1)} + \frac{d\langle\rho^n(4)\rangle}{dJ(1)} \right) \\ &= \mathcal{D}(12) + \int_C d3 \int_C d4 \frac{d\langle\rho^{el}(2)\rangle}{dU_{eff}(3)} V(3-4) \frac{d\langle\rho^n(1)\rangle}{dU(4)} \end{aligned} \quad (\text{F.51})$$

or

$$\int_C d4 \frac{d\langle\rho^n(1)\rangle}{dU(4)} L(42) = \mathcal{D}(12) \quad (\text{F.52})$$

with

$$\begin{aligned} L(12) &= \delta(12) - \int_C d3 V(1-3) \frac{d\langle\rho^{el}(2)\rangle}{dU_{eff}(3)} \\ &= \delta(12) + i\hbar \int_C d3 V(1-3) \frac{dG(22^+)}{dU_{eff}(3)}. \end{aligned} \quad (\text{F.53})$$

Comparing equations (F.42) and (F.53) shows that they are similar, except for the arguments 2 and 3 in $\pi(23) = dG(22^+)/dU_{eff}(3)$, that are exchanged. However, the first order approximation for $\pi(12)$ in equation (F.21) has the property that $\pi(12) = \pi(21)$. One can conclude that $L(12) = \epsilon(12)$. As consequence,

$$\frac{d\langle\rho^n(1)\rangle}{dU(2)} = \int_C d3 \mathcal{D}(13) \epsilon^{-1}(32) \quad (\text{F.54})$$

and the insertion of this result into equation (F.46) gives

$$\begin{aligned} \frac{dU_{eff}(1)}{dU(2)} &= \epsilon^{-1}(12) + \int_C d3 \int_C d4 W(13) \mathcal{D}(34) \epsilon^{-1}(42) \\ &= \epsilon_{eff}^{-1}(12). \end{aligned} \quad (\text{F.55})$$

With this equation, it is possible to compute the total screened potential $W_{eff}(12)$ when carrier-carrier and carrier-phonon interactions are present. Recalling the definition of $W(21)$ in equation (F.10) and replacing the derivate of the effective potential by the value with phonon-interaction yields

$$\begin{aligned} W_{eff}(21) &= \int_C d3 V(1-3) \epsilon_{eff}^{-1}(23) \\ &= W_{el}(21) + \underbrace{\int_C d3 \int_C d4 W_{el}(23) \mathcal{D}(34) W_{el}(41)}_{W_{ph}(21)}. \end{aligned} \quad (F.56)$$

Hence, the presence of carrier-phonon interaction adds a second term $W_{ph}(21)$ to the screened potential $W_{el}(21)$ coming only from carrier-carrier interaction.

F.3.1 Optical Phonon Example

In the second quantization, the Hamiltonian for carrier-optical phonon interaction within the Fröhlich approximation is given by

$$H^{FR} = \int dr \hat{\psi}^\dagger(r) \sum_q \frac{e^{iqr}}{|q|} \left(C a_q + C^* a_{-q}^\dagger \right) \hat{\psi}(r) \quad (F.57)$$

where a_q and a_{-q}^\dagger are the annihilation and creation phonon operators, respectively and

$$C = i \sqrt{\frac{e^2}{V} \frac{\hbar \omega_{LO}}{2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)}. \quad (F.58)$$

C is the Fröhlich constant. Therefore, comparing this Hamiltonian with the Hamiltonian of equation (F.33), one finds

$$H^{FR}(1) = \int d3 V(1-3) \rho^n(3) \quad (F.59)$$

and

$$\rho^n(1) = \int d3 V^{-1}(1-3) H^{FR}(3) \quad (F.60)$$

This results is inserted into equation (F.49) and after some algebra, one finds for $\mathcal{D}(12)$

$$\begin{aligned} \mathcal{D}(12) &= -\frac{i}{\hbar} \frac{\langle T \{ S \Delta \rho^n(2) \Delta \rho^n(1) \} \rangle}{\langle S \rangle} \\ &= \int d3 \int d4 \sum_{q_1 q_2} \frac{|C|^2}{|q_1| |q_2|} e^{iq_1 r_3} e^{iq_2 r_4} V^{-1}(1-3) V^{-1}(2-4) D(q_1 q_2; t_3 t_4) \end{aligned} \quad (F.61)$$

where $D(q_1 q_2; t_3 t_4)$ is the phonon Green's function and is defined as

$$D(q_1 q_2; t_3 t_4) = -\frac{i}{\hbar} \frac{\langle T \{ S A^\dagger(q_1, t_1) A(q_2, t_2) \} \rangle}{\langle S \rangle} \quad (\text{F.62})$$

with $A(q, t) = a_q^\dagger(t) + a_{-q}(t)$. As for the electron Green's function G , there are different phonon Green's function, the lesser, the greater, the retarded, the advanced and so on. One can find an expression for the free phonon Green's functions $D^{(0)}(q, t)$, where $t_1 - t_2 = t$, $q_1 = q_2$ and $S = 1$. In this case, one has

$$\begin{aligned} a_q(t) &= e^{iH_0 t/\hbar} a_q e^{-iH_0 t/\hbar} \\ \langle a_q \rangle &= 0 \end{aligned} \quad (\text{F.63})$$

and therefore [5]

$$\begin{aligned} D_0^>(q, t) &= -\frac{i}{\hbar} [(N_q + 1)e^{-i\omega_q t} + N_q e^{i\omega_q t}] \\ D_0^<(q, t) &= -\frac{i}{\hbar} [(N_q + 1)e^{i\omega_q t} + N_q e^{-i\omega_q t}] \\ D_0^R(q, t) &= -\frac{2}{\hbar} \theta(t) \sin(\omega_q t) \\ D_0^A(q, t) &= \frac{2}{\hbar} \theta(-t) \sin(\omega_q t) \\ &\dots \end{aligned} \quad (\text{F.64})$$

By inserting equation (F.61) into (F.56), an expression is found for the effective potential where carrier-phonon interaction is present

$$\begin{aligned} W_{ph}(21) &= \int_C d3 \int_C d4 \int_C d5 \int_C d6 \sum_{q_1 q_2} \frac{|C|^2}{|q_1||q_2|} e^{iq_1 r_5} e^{iq_2 r_6} W_{el}(23) V^{-1}(3-5) \\ &\quad V^{-1}(4-6) W_{el}(41) D(q_1 q_2; t_5 t_6). \end{aligned} \quad (\text{F.65})$$

According to equation (F.22), the self-energy accounting for carrier-phonon interaction is derived

$$\Sigma^{ph}(12) = i\hbar W_{ph}(21) G(12). \quad (\text{F.66})$$

Further simplifications can be applied if one neglects screening effects in the electronic part of the effective potential, i.e. $W_{el}(21)$ becomes $V(1-2)$. In that case, one has

$$\int_C d3 V(1-3) V(3-2) = \delta(12), \quad (\text{F.67})$$

and the carrier-phonon self-energy is

$$\Sigma^{ph}(12) = i\hbar \sum_{q_1 q_2} \frac{|C|^2}{|q_1||q_2|} e^{iq_1 r_1} e^{iq_2 r_2} D(q_1 q_2; t_1 t_2) G(12). \quad (\text{F.68})$$

Appendix G

Derivation of the Current Equation

G.1 Mathematical Representation

To derive an appropriate equation for the current density $J(x, t)$, one will use the conservation law of quantum mechanical variables after reference [21]. The starting point is the subtraction of equation (2.3) from (2.2), where a general carrier-phonon interaction term of the form $H^{ph} = \int dx \hat{\psi}^\dagger(x) \sum_{\mathbf{q}} e^{i\mathbf{q}x} M(\mathbf{q}) \hat{\psi}(x)$ is added to the total Hamiltonian of (2.1). This gives

$$\begin{aligned}
& i\hbar \left(\frac{d}{dt_1} + \frac{d}{dt_2} \right) G(12) + \frac{\hbar^2}{2m} [(\nabla_{x1} + \nabla_{x2})(\nabla_{x1} - \nabla_{x2})] G(12) = \\
& (U(1) - U(2)) G(12) - i\hbar \int_C d3 (V(1-3) - V(2-3)) G^{(2)}(13^- 23^+) \\
& - \frac{i}{\hbar} \sum_{\mathbf{q}} \frac{C}{\mathbf{q}} (e^{i\mathbf{q}x_1} - e^{i\mathbf{q}x_2}) \langle T \left\{ \hat{\psi}_{\mathcal{H}}(1) (a_{\mathbf{q}} - a_{-\mathbf{q}}^\dagger) \hat{\psi}_{\mathcal{H}}^\dagger(2) \right\} \rangle = \\
& (U(1) - U(2)) G(12) + \int_C d3 (\Sigma^{tot}(13)G(32) - G(13)\Sigma^{tot}(32)). \quad (G.1)
\end{aligned}$$

The last equality results from equations (2.5) and (2.6). By taking the limit $x_2 \rightarrow x_1$ and $t_2 \rightarrow t_1^+$, one obtains

$$i\hbar \frac{d}{dt_1} G^<(x_1 t_1; x_1 t_1) + \nabla_{x_1} \left(\frac{\hbar^2}{2m} \lim_{x_2 \rightarrow x_1} (\nabla_{x1} - \nabla_{x2}) G^<(x_1 t_1; x_2 t_1) \right) = 0. \quad (G.2)$$

Recalling the definition of the carrier density from equation (1.32) yields

$$-\frac{d}{dt_1} n(x_1, t_1) + \nabla_{x_1} \left(\frac{\hbar^2}{2m} \lim_{x_2 \rightarrow x_1} (\nabla_{x1} - \nabla_{x2}) G^<(x_1 t_1; x_2 t_1) \right) = 0. \quad (G.3)$$

This is equivalent to the continuity equation

$$\frac{d}{dt_1} n(x_1, t_1) + \text{div} J(x_1, t_1) = 0, \quad (G.4)$$

where now the current density $J(x_1, t_1)$ is defined by

$$J(x_1, t_1) = \frac{\hbar^2}{2m} \lim_{x_2 \rightarrow x_1} (\nabla_{x_2} - \nabla_{x_1}) G^<(x_1 t_1; x_2 t_1). \quad (\text{G.5})$$

The equivalence of the second and the third equalities of equation (G.1) implies in the limit $x_2 \rightarrow x_1$ and $t_2 \rightarrow t_1^+$ that

$$\int_C d3 \left(\Sigma^{\text{tot}}(x_1 t_1; x_3 t_3) G(x_3 t_3; x_1 t_1) - G(x_1 t_1; x_3 t_3) \Sigma^{\text{tot}}(x_3 t_3; x_1 t_1) \right) = 0. \quad (\text{G.6})$$

The approximation used to calculate the self-energies $\Sigma(12)$ must verify this rule. This is the case for the Hartree, Hartree-Fock, Born, T-matrix, and RPA approximations.

As consequence, the second part of equation (2.93) vanishes and the equation for the current density $J_n(t)$ is simplified.

G.2 Example

In this section, one will prove that the approximation made for carrier-phonon interaction self-energies (see section 2.5.3.2) preserves the current conservation law. For that purpose, the 1-dimensional case is considered and pseudo-Wannier functions centered around one lattice point are chosen as basis. In order that conditions (G.4) and (G.5) are fulfilled, the following equation must be valid (this is just the transformation of (G.6) for the lesser Green's function)

$$\sum_{\mathbf{k}, l} \int \frac{dE}{2\pi} \left(\Sigma_{nl}^R(\mathbf{k}; E) G_{ln}^<(\mathbf{k}; E) + \Sigma_{nl}^<(\mathbf{k}; E) G_{ln}^A(\mathbf{k}; E) - G_{nl}^R(\mathbf{k}; E) \Sigma_{ln}^<(\mathbf{k}; E) - G_{nl}^<(\mathbf{k}; E) \Sigma_{ln}^A(\mathbf{k}; E) \right) = 0. \quad (\text{G.7})$$

The self-energies $\Sigma^R(\mathbf{k}; E)$, $\Sigma^<(\mathbf{k}; E)$, and $\Sigma^A(\mathbf{k}; E)$ are given in equation (2.65). Due to the pseudo-Wannier functions basis, the matrix element $M_{n_1 n_2}(\mathbf{q})$ can be written as

$$M_{n_1 n_2}(\mathbf{q}) = \left| \frac{C}{\mathbf{q}} \right| e^{iq_z(z_{n_1} - z_{n_2})}. \quad (\text{G.8})$$

Taking a look at the form of equation (G.7) and of the self-energies, one sees that the term $G_{nl}^R(\mathbf{k}; E) \Sigma_{ln}^<(\mathbf{k}; E)$ can compensate one part of $\Sigma_{nl}^R(\mathbf{k}; E) G_{ln}^<(\mathbf{k}; E)$ for each different index l

$$\begin{aligned} \sum_{\mathbf{k}, \mathbf{q}} \int \frac{dE}{2\pi} \left| \frac{C}{\mathbf{q}} \right|^2 & \left(e^{iq_z(z_n - z_l)} \left[(N_{\mathbf{q}} + 1) G_{nl}^<(\mathbf{k} - \mathbf{q}_{||}; E - \hbar\omega_{\mathbf{q}}) + N_{\mathbf{q}} G_{nl}^<(\mathbf{k} - \mathbf{q}_{||}; E + \hbar\omega_{\mathbf{q}}) \right] G_{ln}^<(\mathbf{k}; E) \right. \\ & \left. - G_{nl}^<(\mathbf{k}; E) e^{iq_z(z_l - z_n)} \left[N_{\mathbf{q}} G_{ln}^<(\mathbf{k} - \mathbf{q}_{||}; E - \hbar\omega_{\mathbf{q}}) + (N_{\mathbf{q}} + 1) G_{ln}^<(\mathbf{k} - \mathbf{q}_{||}; E + \hbar\omega_{\mathbf{q}}) \right] \right). \end{aligned}$$

One immediately sees that this term is equal to zero if one makes some variable transformations: first, in the second line \mathbf{q} is replaced by $-\mathbf{q}'$ (sum over \mathbf{q}' instead of \mathbf{q}) and thus $\mathbf{k} + \mathbf{q}'_{||}$ by \mathbf{k}' (sum over \mathbf{k}' , $G_{nl}^<(\mathbf{k}; E) \rightarrow G_{nl}^<(\mathbf{k}' - \mathbf{q}'_{||}; E)$). Then, still for the second line, the terms depending on $N_{\mathbf{q}}$ and $N_{\mathbf{q}} + 1$ must be treated separately:

- $E - \hbar\omega_{\mathbf{q}}$ becomes E' , the integral over E an integral over E' , and the Green's function $G_{nl}^<(\mathbf{k}' - \mathbf{q}'_{||}; E) \rightarrow G_{nl}^<(\mathbf{k}' - \mathbf{q}'_{||}; E' + \hbar\omega_{\mathbf{q}})$. This term is canceled by the second one of the first line.
- $E + \hbar\omega_{\mathbf{q}}$ is replaced by E' , the integral over E by an integral over E' , and finally $G_{nl}^<(\mathbf{k}' - \mathbf{q}'_{||}; E) \rightarrow G_{nl}^<(\mathbf{k}' - \mathbf{q}'_{||}; E' - \hbar\omega_{\mathbf{q}})$. This term is equivalent to the first term in the first line and disappears as consequence.

With the variable transformation procedure, it can be proved that all the terms present in equation (G.7) are canceled by each other and that the current conservation law is satisfied. Condition (G.7) must hold for all types of interactions and all the approximations made for the self-energies.

Appendix H

Initial Correlations

H.1 Introduction

In this section, the case where initial correlations are present in the definition of the Green's function will be treated [22, 23]. This is an important effect if one wants to simulate the transient behavior of a device. For steady state transport, it appears plausible that the initial correlations have been washed out by the interactions when one reaches the steady state. One starts with the expression for the Green's function $G(11')$

$$G(11') = -\frac{i}{\hbar} \frac{\text{tr} \left(\rho(t_0) T \left\{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\} \right)}{\text{tr}(\rho(t_0))}. \quad (\text{H.1})$$

$\rho(t_0)$ describes the initial state of the system and contains one- and two- particle operators

$$\rho(t_0) = e^{-B} = e^{-(B^{(0)} + B^{(1)})}, \quad (\text{H.2})$$

where $B^{(0)}$ is a one-particle operator and $B^{(1)}$ a two-particle one with

$$B = \int dx \hat{\psi}^\dagger(x) \lambda^{(1)}(x) \hat{\psi}(x) + \frac{1}{2} \int dx \int dy \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \lambda^{(2)}(x, y) \hat{\psi}(y) \hat{\psi}(x).$$

In equation (H.1), the creation and annihilation operators $\hat{\psi}_H(x, t)$ and $\hat{\psi}_H^\dagger(x', t')$ are given in the Heisenberg picture and are governed by the Hamiltonian $H = H^{(0)} + H^{(1)}$, where $H^{(0)}$ is a one-particle operator and $H^{(1)}$ a two-particle operator, as for B with

$$H = \int dx \hat{\psi}^\dagger(x) \left(-\frac{\hbar^2 \nabla_x^2}{2m} \right) \hat{\psi}(x) + \frac{1}{2} \int dx \int dy \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) V(x - y) \hat{\psi}(y) \hat{\psi}(x).$$

There are two crucial points with the definition of the Green's function in equation (H.1):

- the time-development operators for $\hat{\psi}_H^\dagger$ and $\hat{\psi}_H$ involve many-particle contributions via the Hamiltonian H

- $\rho(t_0)$ is a many-particle density matrix due to $\lambda^{(2)}$.

However, to apply Wick's theorem, one has to work with noninteracting operators and a non-correlated initial density matrix $\rho(t_0)$. Therefore, the definition of the Green's function must be adapted to meet these two statements. First of all, $\rho(t_0)$ can be rewritten as

$$\rho(t_0) = e^{-B} = e^{Bx_0} e^{-B^{(0)}x_0} e^{-B^{(0)}} e^{B^{(0)}(x_0+1)} e^{-B(x_0+1)} \quad (\text{H.3})$$

with $-1 \leq x_0 \leq 0$. One defines two new quantities, $U_1(\tau) = e^{B^{(0)}\tau} e^{-B\tau}$ with $\tau > 0$ and its parent $U_2(\tau) = e^{B\tau} e^{-B^{(0)}\tau}$ where $\tau < 0$. With some algebra similar to Appendix A, one finds for $U_1(\tau)$

$$U_1(\tau)|_{\tau>0} = T^c \left\{ \exp \left(- \int_0^\tau d\tau' B_I^{(1)}(\tau') \right) \right\}. \quad (\text{H.4})$$

For $U_2(\tau)$, the procedure is the same as in Appendix B, except that T^a is replaced by T^c because τ is smaller than 0.

$$\begin{aligned} U_2(\tau)|_{\tau<0} &= T^c \left\{ \exp \left(\int_0^\tau d\tau' B_I^{(1)}(\tau') \right) \right\} \\ &= T^c \left\{ \exp \left(- \int_\tau^0 d\tau' B_I^{(1)}(\tau') \right) \right\}. \end{aligned} \quad (\text{H.5})$$

The index I in $B_I^{(1)}(\tau')$ represents a time evolution in the interaction picture

$$B_I^{(1)}(\tau') = e^{\tau' B^{(0)}} B^{(1)} e^{-\tau' B^{(0)}}. \quad (\text{H.6})$$

Obviously, the definitions for U_1 and U_2 are identical and one can introduce an evolution operator $S_I^B(\tau_1, \tau_2)$ (I because interaction picture and B because relative to the B operator) with

$$S_I^B(\tau_1, \tau_2)|_{\tau_1>\tau_2} = T^c \left\{ \exp \left(- \int_{\tau_2}^{\tau_1} d\tau' B_I^{(1)}(\tau') \right) \right\} \quad (\text{H.7})$$

and relate it to U_1 and U_2

$$U_1(\tau)|_{\tau>0} = S_I^B(\tau, 0), \quad U_2(\tau)|_{\tau<0} = S_I^B(0, \tau). \quad (\text{H.8})$$

These results are inserted in the definition of the Green's function

$$\begin{aligned} G(11') &= -\frac{i}{\hbar} \frac{\text{tr} \left(S_I^B(0, x_0) e^{-B^{(0)}} S_I^B(x_0 + 1, 0) T \left\{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\} \right)}{\text{tr} \left(S_I^B(0, x_0) e^{-B^{(0)}} S_I^B(x_0 + 1, 0) \right)} \\ &= -\frac{i}{\hbar} \frac{\langle S_I^B(x_0 + 1, 0) T \left\{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\} S_I^B(0, x_0) \rangle_0}{\langle S_I^B(x_0 + 1, x_0) \rangle_0}. \end{aligned} \quad (\text{H.9})$$

The second line is obtained because of the cyclic property of the trace operator. It remains to change the time evolution of the creation and annihilation operators to ensure that they are noninteracting

$$\begin{aligned}\hat{\psi}_H(x, t) &= S_I^H(t_0, t) \hat{\psi}_I(x, t) S_I^H(t, t_0) \\ \hat{\psi}_H^\dagger(x', t') &= S_I^H(t_0, t') \hat{\psi}_I^\dagger(x', t') S_I^H(t', t_0)\end{aligned}\quad (\text{H.10})$$

where one has for the time evolution S_I^H in the interaction picture and relative to H

$$S_I^H(t, t') = T^v \left\{ \exp \left(-\frac{i}{\hbar} \int_{t'}^t dt_1 H_I^{(1)}(t_1) \right) \right\}, \quad \text{with } v = \begin{cases} c, & t > t' \\ a, & t' > t \end{cases}$$

and

$$H_I^{(1)}(t_1) = e^{iH^{(0)}/\hbar} H^{(1)} e^{-iH^{(0)}/\hbar} \quad (\text{H.11})$$

The second requirement of Wick's theorem is therefore fulfilled and the modifications of the operators given in the Heisenberg picture can be included in the definition of the Green's function

$$G(11') = -\frac{i}{\hbar} \frac{\langle S_I^B(x_0 + 1, 0) T_C \left\{ \exp \left(-\frac{i}{\hbar} \int_C dt_1 H_I^{(1)}(t_1) \right) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \right\} S_I^B(0, x_0) \rangle_0}{\langle S_I^B(x_0 + 1, x_0) \rangle_0},$$

where the operator T_C orders the time along the contour C from Figure 1.1, for example. The twofold expansion of the initial density matrix and the time-development of the creation and annihilation operators may conveniently be combined to one single expansion. To this end one utilizes the striking similarity between the treatment of the initial density matrix and the time-development operators, both of which are exponential functions. One defines a contour \underline{C} , which elongates C in Figure 1.1 to take account of the parts going from x_0 to 0 and from 0 to $x_0 + 1$. To reduce the complexity of the problem, x_0 is set to 0 and one obtains the contour in Figure H.1. Then one introduces an imaginary time $\xi = (t, \tau)$, where t is the

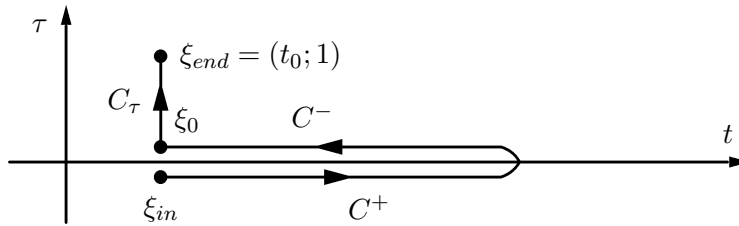


Figure H.1: Contour \underline{C} for the evaluation of the Green's function with initial correlations. This is the special case, where x_0 is equal to 0

real part of the time and τ the imaginary one. ξ goes along the contour \underline{C} from Figure H.1. The new time-ordering operator $T_{\underline{C}}$ orders the elements of the Green's function along \underline{C} . Hence a point on $C = C^+ + C^-$ is always “earlier” than a point

on C_τ .

Furthermore, one defines an interaction picture with respect to

$$\underline{H}_I^{(1)}(\xi) = \begin{cases} H_I^{(1)}(t), & \xi \text{ on } C \\ -i\hbar B_I^{(1)}(\tau), & \xi \text{ on } C_\tau \end{cases} \quad (\text{H.12})$$

which is a combination of the interaction pictures defined in equations (H.6) and (H.11). Finally, one collects the expansion of the initial density matrix $\rho(t_0)$ and the time-development operator and insert it into equation (H.1) for the Green's function

$$G(11') = -\frac{i}{\hbar} \frac{\langle T_{\underline{C}} \left\{ \exp \left(-\frac{i}{\hbar} \int_{\underline{C}} d\xi \underline{H}_I^{(1)}(\xi) \right) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \right\} \rangle_0}{\langle T_{\underline{C}} \left\{ \exp \left(-\frac{i}{\hbar} \int_{\underline{C}} d\xi \underline{H}_I^{(1)}(\xi) \right) \right\} \rangle_0}. \quad (\text{H.13})$$

The contour C_τ of the denominator was elongated with C to form \underline{C} .

Wick's theorem is valid for equation (H.13) because firstly the average is taken over a one-particle density matrix $\rho(t_0) = e^{-B^{(0)}}$ and secondly, all operators are given in an interaction picture corresponding to a non-interacting system. Unfortunately, the application of Wick's theorem immediately reveals that such an expression for $G(11')$ will contain contractions of operators for which one is a real-time operator and the other an imaginary-time operator. This means that for real-time functions $G(11')$ the system of equations is not closed because $\underline{H}_I^{(1)}$ is defined on the contour \underline{C} . Therefore, one has to continue $G(11')$ to \underline{C} and one obtains the \underline{C} -contour-ordered mixed Green's function $\underline{G}(11')$, which means that the time argument of \underline{G} are on the contour \underline{C}

$$\underline{G}(11') = -\frac{i}{\hbar} \frac{\langle T_{\underline{C}} \left\{ \exp \left(-\frac{i}{\hbar} \int_{\underline{C}} d\xi \underline{H}_I^{(1)}(\xi) \right) \hat{\psi}_I(1) \hat{\psi}_I^\dagger(1') \right\} \rangle_0}{\langle T_{\underline{C}} \left\{ \exp \left(-\frac{i}{\hbar} \int_{\underline{C}} d\xi \underline{H}_I^{(1)}(\xi) \right) \right\} \rangle_0}. \quad (\text{H.14})$$

Because Wick's theorem holds exactly for equation (H.14), the equations of motion for $\underline{G}(11')$ can be derived with the procedure outlined in the first chapter and in Appendix F.

H.2 Equations of Motion

To derive the equations of motion for $\underline{G}(11')$, one starts with its definition in the Heisenberg picture, without the expansion for the initial density matrix

$$\underline{G}(11') = -\frac{i}{\hbar} \langle T_{\underline{C}} \left\{ \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \right\} \rangle. \quad (\text{H.15})$$

The equation of motion for $\underline{G}(11')$ follows directly the equation of motion for the field operators $\hat{\psi}_H(1)$ and $\hat{\psi}_H^\dagger(1')$ in the Heisenberg picture on the extended contour

C. For an operator $O_H^B(\tau) = e^{\tau B} O e^{-\tau B}$ in the Heisenberg picture relative to the imaginary time τ and the operator B , one has

$$i\hbar \frac{d}{d\tau} O_H^B(\tau) = [O_H^B(\tau), -i\hbar B_H^B(\tau)] \quad (\text{H.16})$$

and for an operator $O_H^H(t) = e^{itH/\hbar} O e^{-itH/\hbar}$ also in the Heisenberg picture, but for real time t and with respect to the operator H

$$i\hbar \frac{d}{dt} O_H^H(t) = [O_H^H(t), H_H^H(t)]. \quad (\text{H.17})$$

As in the last section, one defines a common Heisenberg picture with respect to

$$\underline{O}_H(\xi) = \left\{ \begin{array}{ll} O_H^H(t), & \xi \text{ on } C \\ -i\hbar O_H^B(\tau), & \xi \text{ on } C_\tau \end{array} \right| \quad \underline{H}_H(\xi) = \left\{ \begin{array}{ll} H_H^H(t), & \xi \text{ on } C \\ -i\hbar B_H^B(\tau), & \xi \text{ on } C_\tau \end{array} \right.$$

and a common equation of motion

$$i\hbar \frac{d}{d\xi} \underline{O}_H(\xi) = [\underline{O}_H(\xi), \underline{H}_H(\xi)]. \quad (\text{H.18})$$

Furthermore $\underline{H}_H(\xi)$ is defined as

$$\begin{aligned} \underline{H}_H(\xi) &= \int dx \, \hat{\psi}_H^\dagger(x, \xi) \underline{h}(x, \xi) \hat{\psi}_H(x, \xi) \\ &\quad + \frac{1}{2} \int dx \int dy \, \hat{\psi}_H^\dagger(x, \xi) \hat{\psi}_H^\dagger(y, \xi) \underline{V}(x, \xi; y, \xi) \hat{\psi}_H(y, \xi) \hat{\psi}_H(x, \xi). \end{aligned}$$

with

$$\underline{h}(x, \xi) = \left\{ \begin{array}{ll} -\frac{\hbar^2 \nabla_x^2}{2m}, & \xi \text{ on } C \\ -i\hbar \lambda^{(1)}(x), & \xi \text{ on } C_\tau \end{array} \right| \quad \underline{V}(x, \xi; y, \xi) = \left\{ \begin{array}{ll} V(x - y), & \xi \text{ on } C \\ -i\hbar \lambda^{(2)}(x, y), & \xi \text{ on } C_\tau. \end{array} \right.$$

To find the paired equations of motion for the mixed Green's function $\underline{G}(11')$, one has to solved both of the following equations

$$i\hbar \frac{d}{d\xi} \hat{\psi}_H(1) = [\hat{\psi}_H(1), \underline{H}_H(\xi)], \quad i\hbar \frac{d}{d\xi'} \hat{\psi}_H^\dagger(1') = [\hat{\psi}_H^\dagger(1'), \underline{H}_H(\xi')],$$

where one will concentrate on the first equation

$$\begin{aligned} i\hbar \frac{d}{d\xi} \hat{\psi}_H(x, \xi) &= \underline{h}(x, \xi) \hat{\psi}_H(x, \xi) + \frac{1}{2} \int dy \, \underline{V}(x, \xi; y, \xi) \hat{\psi}_H^\dagger(y, \xi) \hat{\psi}_H(y, \xi) \hat{\psi}_H(x, \xi) \\ &\quad - \frac{1}{2} \int dy \, \underline{V}(y, \xi; x, \xi) \hat{\psi}_H^\dagger(y, \xi) \hat{\psi}_H(x, \xi) \hat{\psi}_H(y, \xi) \\ &= \underline{h}(x, \xi) \hat{\psi}_H(x, \xi) + \int dy \, \underline{V}(x, \xi; y, \xi) \hat{\psi}_H^\dagger(y, \xi) \hat{\psi}_H(y, \xi) \hat{\psi}_H(x, \xi). \end{aligned}$$

The third line is obtained because of the symmetry properties of \underline{V}

$$\underline{V}(x, \xi; y, \xi) = \underline{V}(y, \xi; x, \xi). \quad (\text{H.19})$$

Recalling the definition of the mixed Green's function $\underline{G}(11')$ in equation (H.15) and using the relationship derived above, one finds the mixed equation of motion on contour \underline{C} from Figure H.1

$$\left(i\hbar \frac{d}{d\xi} + \underline{h}(1)\right) \underline{G}(11') = \underline{\delta}(11') - i\hbar \int_{\underline{C}} d2 \underline{V}(12) \underline{G}^{(2)}(121'2), \quad (\text{H.20})$$

where

$$\underline{V}(12) = \underline{V}(x_1, \xi_1; x_2, \xi_1) \delta(\xi_1 - \xi_2), \quad (\text{H.21})$$

and

$$\underline{G}^{(2)}(121'2') = \left(-\frac{i}{\hbar}\right)^2 \langle T_{\underline{C}} \{ \underline{\psi}_H(1) \underline{\psi}_H(2) \underline{\psi}_H^\dagger(2') \underline{\psi}_H^\dagger(1') \} \rangle. \quad (\text{H.22})$$

As for the real-time Green's function $G(11')$, one can introduce a self-energy $\underline{\Sigma}(11')$ for the mixed $\underline{G}(11')$. It is given by

$$\underline{\Sigma}(11') = -i\hbar \int_{\underline{C}} d2 \int_{\underline{C}} d3 \underline{V}(12) \underline{G}^{(2)}(1232) \underline{G}^{-1}(31') \quad (\text{H.23})$$

To find analytical expressions for $\underline{\Sigma}(11')$, the same procedure as described in Appendix F can be used. Furthermore, the inverse mixed free Green's function $\underline{G}_0^{-1}(12)$ corresponding to equation (2.10) is defined as

$$\underline{G}_0^{-1}(12) = \left(i\hbar \frac{d}{d\xi_1} + \underline{h}(1)\right) \underline{\delta}(12). \quad (\text{H.24})$$

H.3 Dyson Equation on the Extended Contour

Collecting all the previous equations, one sees that the mixed Green's function $\underline{G}(11')$ satisfies the Dyson equation on the extended contour \underline{C} (Figure H.1). This equation and its adjoint can be written in the form

$$\begin{aligned} \int_{\underline{C}} d2 \underline{G}_0^{-1}(12) \underline{G}(21') &= \underline{\delta}(11') + \int_{\underline{C}} d2 \underline{\Sigma}(12) \underline{G}(21') \\ \int_{\underline{C}} d2 \underline{G}(12) \underline{G}_0^{-1}(21') &= \underline{\delta}(11') + \int_{\underline{C}} d2 \underline{G}(12) \underline{\Sigma}(21'). \end{aligned} \quad (\text{H.25})$$

The difference between the mixed Green's functions $\underline{G}(11')$ and the usual real-time (on part C of the contour \underline{C}) and thermodynamic Green's functions (on part C_τ of \underline{C}) is conveniently illustrated by expressing $\underline{G}(11')$ in terms of its components. With the definition of the contour \underline{C} from Figure H.1, one writes

$$\underline{G}(11') = \begin{cases} G(11') = -\frac{i}{\hbar} \langle T \{ \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \} \rangle, & 1, 1' \text{ on } C, \\ \mathcal{G}^>(11') = -\frac{i}{\hbar} \langle \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \rangle, & 1 \text{ on } C_\tau, 1' \text{ on } C, \\ \mathcal{G}^<(11') = \frac{i}{\hbar} \langle \hat{\psi}_H^\dagger(1') \hat{\psi}_H(1) \rangle, & 1 \text{ on } C, 1' \text{ on } C_\tau, \\ \frac{i}{\hbar} \mathcal{G}(11') = -\frac{i}{\hbar} \langle T_\tau \{ \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') \} \rangle, & 1, 1' \text{ on } C_\tau, \end{cases} \quad (\text{H.26})$$

where $G(11')$ and $\mathcal{G}(11')$ are the real-time Green's function from equation (1.41) and the thermodynamic Green's function from (1.11), respectively. One also has to consider the “cross Green's functions” $\mathcal{G}^<(11')$ and $\mathcal{G}^>(11')$, which are constructed from Heisenberg operators with different types of evolution. These functions satisfy the obvious boundary conditions

$$\begin{aligned} \mathcal{G}^>(11')|_{t'=t_0} &= \frac{i}{\hbar} \mathcal{G}(11')|_{\tau'=0}, & \mathcal{G}^<(11')|_{t=t_0} &= \frac{i}{\hbar} \mathcal{G}(11')|_{\tau=0}, \\ \mathcal{G}^>(11')|_{\tau=0} &= G^>(11')|_{t=t_0}, & \mathcal{G}^<(11')|_{\tau'=0} &= G^<(11')|_{t'=t_0}, \end{aligned}$$

which relate them to the thermodynamic and real-time Green's functions. Secondly, the operator $\underline{G}_0^{-1}(11')$ from equation (H.24) is defined as

$$\underline{G}_0^{-1}(11') = \begin{cases} G_0^{-1}(11') = \left(i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_x^2}{2m} \right) \delta(t, t') \delta(x - x'), & 1, 1' \text{ on } C \\ -i\hbar \mathcal{G}_0^{-1}(11') = i\hbar \left(\frac{d}{d\tau} + \lambda^{(1)}(x) \right) \delta(\tau - \tau') \delta(x - x'), & 1, 1' \text{ on } C_\tau \\ 0, & \text{otherwise.} \end{cases}$$

Finally, the components of the self-energy $\underline{\Sigma}(11')$ from equation (H.23) will be denoted by

$$\underline{\Sigma}(11') = \begin{cases} \Sigma(11'), & 1, 1' \text{ on } C, \\ \mathcal{K}^<(11'), & 1 \text{ on } C, 1' \text{ on } C_\tau, \\ \mathcal{K}^>(11'), & 1 \text{ on } C_\tau, 1' \text{ on } C, \\ -i\hbar \mathcal{K}(11'), & 1, 1' \text{ on } C_\tau, \end{cases}$$

where $\Sigma(11')$ contains $\Sigma^{\geq}(11')$ and $\Sigma^{R,A}(11')$.

H.3.1 Real-Time Components of the Mixed Green's Function

If 1 and 1' in equation (H.25) correspond to the real part C of the contour \underline{C} from Figure H.1, one has, since the part C_τ is later along \underline{C} than C (only the first equation will be considered for each case)

$$\begin{aligned} \left(i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G(11') &= \delta(11') + \int_C d2 \Sigma(12) G(21') \\ &\quad + \int_{C_\tau} d2 \mathcal{K}^<(12) \mathcal{G}^>(21'). \end{aligned} \quad (\text{H.27})$$

Recalling the Langreth theorem from section 2.3, one obtains for the different components of $G(11')$

$$\begin{aligned} \left(i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G^{\geq}(11') &= \int_{t_0}^{\infty} d2 \Sigma^R(12) G^{\geq}(21') + \int_{t_0}^{\infty} d2 \Sigma^{\geq}(12) G^A(21') \\ &\quad + \int_{C_\tau} d2 \mathcal{K}^<(12) \mathcal{G}^>(21') \end{aligned} \quad (\text{H.28})$$

and

$$\left(i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G^{R,A}(11') = \int_{t_0}^{\infty} d2 \Sigma^{R,A}(12) G^{R,A}(21') \quad (\text{H.29})$$

with $\int_{t_0}^{\infty} d2 = \int_{t_0}^{\infty} dt_2 \int dx_2$.

It is obvious that the integration over C_τ disappears for the Dyson equation of $G^{R,A}(11')$ because of the relationship defined in equation (1.26).

H.3.2 Thermodynamic Component of the Mixed Green's Function

Starting again with equation (H.25), one places 1 and 1' on the part C_τ of the contour \underline{C} (Figure H.1). Thus one arrives at equation

$$\begin{aligned} \int_{C_\tau} d2 (\mathcal{G}_0^{-1}(12) - \mathcal{K}(12)) \mathcal{G}(21') &= \delta(11') + \int_C d2 \mathcal{K}^>(12) \mathcal{G}^<(21') \\ &= \delta(11') + \int_{t_0}^{\infty} d2 \mathcal{K}^>(12) \mathcal{G}^<(21') \\ &\quad - \int_{t_0}^{\infty} d2 \mathcal{K}^>(12) \mathcal{G}^<(21') \\ &= \delta(11') \end{aligned} \quad (\text{H.30})$$

The second term on the right-hand side of the first line of equation (H.30) vanishes because the values of $\mathcal{K}^>(12)$ and $\mathcal{G}^<(21')$ do not depend if the time argument of 2 corresponds to the chronological (C^+) or anti-chronological (C^-) branch of the contour from Figure H.1. Therefore, one sees that the thermodynamic component of $\underline{\mathcal{G}}(11')$ satisfies a Dyson equation which is not connected with other Green's functions. This is only true as long as the self-energy $\mathcal{K}(12)$ is not connected with the real-time evolution of the system.

H.3.3 Cross Components of the Mixed Green's Function

To complete the set of Green's function being part of $\underline{\mathcal{G}}(11')$, one derives the equations of motion for the cross components \mathcal{G}^{\geq} . In equation (H.25), 1 is now on the C part of the contour \underline{C} and 1' on C_τ . Hence one obtains

$$\int_C d2 (G_0^{-1}(12) - \Sigma(12)) \mathcal{G}^<(21') = \frac{i}{\hbar} \int_{C_\tau} d2 \mathcal{K}^<(12) \mathcal{G}(21'). \quad (\text{H.31})$$

With the definitions of $\Sigma(12)$ given in [11]

$$\begin{aligned} \Sigma(12) &= \Sigma^\delta + \theta(t_1, t_2) \Sigma^>(12) + \theta(t_2, t_1) \Sigma^<(12) \\ \Sigma^R(12) &= \Sigma^\delta + \theta(t_1 - t_2) (\Sigma^>(12) - \Sigma^<(12)), \end{aligned}$$

where Σ^δ is the time-independent Hartree-Fock part of the self-energy defined in equation (F.26). Therefore, whatever the branch on which the time argument t_1 is, it can easily be checked that in both cases, one gets the same equation

$$\int_C d2 G_0^{-1}(12) \mathcal{G}^<(21') = \int_{t_0}^{\infty} d2 \Sigma^R(12) \mathcal{G}^<(21') + \frac{i}{\hbar} \int_{C_\tau} d2 \mathcal{K}^<(12) \mathcal{G}(21').$$

This equation describes the evolution of $\mathcal{G}^<(11') = \mathcal{G}^<(x, t; x', \tau')$ with respect to its real-time argument t . To derive the equation describing the imaginary evolution

of $\mathcal{G}^<(11')$, one uses the second equation in (H.25), still with 1 on the C part of the contour \underline{C} and 1' on C_τ

$$\int_{C_\tau} d2 \mathcal{G}^<(12) (\mathcal{G}_0^{-1}(21') - \mathcal{K}(21')) = \frac{i}{\hbar} \int_{t_0}^{\infty} d2 G^R(12) \mathcal{K}^<(21'). \quad (\text{H.32})$$

The analogous procedure can be repeated for $\mathcal{G}^>(11')$. The results are given in [22].

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