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 one 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

\[ G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle \Psi_0 | T_c \{ \hat{\psi}_H(x, t) \hat{\psi}_H^\dagger(x', t') \} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \]  

(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-term 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

$$T^c\{A(t1)B(t2)C(t3)\} = C(t3)A(t1)B(t2) \quad (1.3)$$

if $t3 > t1 > t2$. 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 $\hat{\psi}^\dagger_H(x', t')$ 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 $\phi_k$, 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 $\langle \Psi_0|\Psi_0\rangle$ 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
1.2 Equilibrium Green’s Functions at Zero Temperature

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

\[
G(x, t; x', t') = -\frac{i}{\hbar} \langle \phi_0 | S(-\infty, 0) T^c \{ \hat{\psi}_H(x, t) \hat{\psi}^\dagger_H(x', t') \} S(0, -\infty) | \phi_0 \rangle
\]

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

\[
\langle \phi_0 | S(-\infty, 0) T^c \{ S(0, t) \hat{\psi}_I(x, t) S(t, 0) S(0, t') \hat{\psi}^\dagger_I(x', t') \} S(t', 0) S(0, -\infty) | \phi_0 \rangle
\]

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 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 \(\phi_k(x) = e^{ikx}/\sqrt{V}\), one gets for the free Green’s function

\[
G_0(x, t; x', t') = -\frac{i}{\hbar} \sum_{kk'} \frac{e^{i(kx - k'x')}}{V} \langle \phi_0 | T \{ c_k(t) c_k^\dagger(t') \} | \phi_0 \rangle
\]

\[
= -\frac{i}{\hbar} \sum_k \frac{e^{ik(x - x')}}{V} \langle \phi_0 | T \{ e^{iH_0t/\hbar} c_k e^{-iH_0(t - t')/\hbar} c_k^\dagger e^{-iH_0t'/\hbar} \} | \phi_0 \rangle
\]

\[
= -\frac{i}{\hbar} \sum_k \frac{e^{ik(x - x')}}{V} \langle \phi_0 | c_k c_k^\dagger | \phi_0 \rangle T \{ e^{-iE_k(t - t')/\hbar} \}
\]

\[
= G_0(x - x'; t - t').
\]

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

\[
G_0(k, \omega) = \int dx \int dt \ e^{-ikx} e^{i\omega t} G_0(x; t)
\]
becomes stands for the trace. Then, the one-particle Green’s function at finite temperature
\[ G(x, t; x', t') = \frac{-i}{\hbar} \sum_{k'} \int dx \frac{e^{-ix(k-k')}}{V} \left( \int_0^\infty dt \ e^{i(\omega-E_k/\hbar+in)t} \langle \phi_0 | c_{k'}^\dagger c_k | \phi_0 \rangle \right. \\
- \left. \int_{-\infty}^0 dt \ e^{i(\omega-E_k/\hbar-in)t} \langle \phi_0 | c_{k'}^\dagger c_k | \phi_0 \rangle \right) \\
= \frac{1 - f_k}{\hbar \omega - E_k + i\eta} + \frac{f_k}{\hbar \omega - E_k - i\eta}. \tag{1.9} \]
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 \( \mu \) and 0 otherwise. The constant \( \eta \), 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, \( \mu \) the chemical potential, \( K = H - \mu N \), \( \beta \) the inverse temperature and the symbol \( \text{tr} \) stands for the trace. Then, the one-particle Green’s function at finite temperature becomes
\[ G(x, t; x', t') = \frac{-i}{\hbar} \text{tr} \left( e^{-\beta K T^c} \{ \hat{\psi}(x, t) \hat{\psi}^\dagger (x', t') \} \right) \frac{\text{tr} (e^{-\beta K})}{\text{tr} (e^{-\beta K})} \\
= \frac{-i}{\hbar} \text{tr} \left( e^{-\beta K T^c} \{ e^{iKt/\hbar} \hat{\psi}(x) e^{-iK(t-t')/\hbar} \hat{\psi}^\dagger (x') e^{-iK't'/\hbar} \} \right) \frac{\text{tr} (e^{-\beta K})}{\text{tr} (e^{-\beta K})} \\
= \frac{-i}{\hbar} \text{tr} \left( e^{-\beta K T^c} \{ e^{iK(t-t')/\hbar} \hat{\psi}(x) e^{-iK(t-t')/\hbar} \hat{\psi}^\dagger (x') \} \right) \frac{\text{tr} (e^{-\beta K})}{\text{tr} (e^{-\beta K})}. \tag{1.11} \]
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 \( e^{-iK(t-t')/\hbar} \). The Green’s function \( G(x, t; x', t') \) then becomes \( G(x - x', t - t') \) and the coordinate...
1.3 Equilibrium Finite Temperature Green’s Functions

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

$$G(k, t) = -i \frac{\hbar}{h} \text{tr} \left( e^{-\beta K T^c} \left\{ e^{iKt/h} c_k e^{-iKt/h} c_k^\dagger \right\} \right) \text{tr} \left( e^{-\beta K} \right).$$  \hspace{1cm} (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 $G(k, \tau)$.

### 1.3.1 Matsubara Green’s Functions

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

$$G(k, \tau) = -i \frac{\hbar}{h} \text{tr} \left( e^{-\beta (H - \mu N) T_\tau} \left\{ e^{\tau (H - \mu N)/h} c_k e^{-\tau (H - \mu N)/h} c_k^\dagger \right\} \right) \text{tr} \left( e^{-\beta (H - \mu N)} \right)$$

$$= -\frac{1}{\hbar} \text{tr} \left( e^{-\beta K T_\tau} \left\{ c_k(\tau) c_k^\dagger \right\} \right) \text{tr} \left( e^{-\beta K} \right). \hspace{1cm} (1.13)$$

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

- $\tau$ must be smaller than $\hbar/\beta$ otherwise the convergence of the trace is not assured.

- $G(k, \tau)$ is antisymmetric on the interval $-\hbar/\beta < \tau < \hbar/\beta$ for Fermions. This is due to the cyclic property of the trace. Considering a $\tau$ between 0 and $\hbar/\beta$, one has

$$G(k, \tau) = -\frac{1}{\hbar} \text{tr} \left( e^{-\beta (H - \mu N) \tau} c_k(\tau) c_k^\dagger \right) \text{tr} \left( e^{-\beta (H - \mu N)} \right)$$

$$= -\frac{1}{\hbar} \text{tr} \left( c_k^\dagger e^{-\beta (H - \mu N) \tau} c_k(\tau) \right) \text{tr} \left( e^{-\beta (H - \mu N)} \right)$$

$$= -\frac{1}{\hbar} \text{tr} \left( e^{-\beta (H - \mu N) \tau} c_k^\dagger e^{-\beta (H - \mu N) \tau} c_k(\tau) e^{\beta (H - \mu N) \tau} \right) \text{tr} \left( e^{-\beta (H - \mu N)} \right)$$

$$= -G(k, \tau - \hbar/\beta) \hspace{1cm} (1.14)$$
and for $-\hbar \beta < \tau < 0$
\[
G(k, \tau) = -G(k, \tau + \hbar \beta).
\] (1.15)

This last property suggests a Fourier series expansion in the strip $[-\hbar \beta, \hbar \beta]$
\[
G(k, \tau) = \sum_n c_n e^{-i\omega_n \tau}
\] (1.16)
with $\omega_n = \frac{(2n+1)\pi}{\hbar \beta}$ for Fermions and
\[
c_n = \frac{1}{T} \int_{-T/2}^{T/2} d\tau \ G(k, \tau) e^{i\omega_n \tau} = \frac{1}{2\hbar \beta} \int_{-\hbar \beta}^{\hbar \beta} d\tau \ G(k, \tau) e^{i\omega_n \tau} = \frac{1}{\hbar \beta} \int_0^{\hbar \beta} d\tau \ G(k, \tau) e^{i\omega_n \tau}.
\]

Defining $G(k, i\omega_n) = \hbar \beta c_n$ implies for the Fourier series that
\[
G(k, \tau) = \frac{1}{\hbar \beta} \sum_n G(k, i\omega_n) e^{-i\omega_n \tau}.
\] (1.17)

It still remains to find a perturbation expansion for the Matsubara Green’s function $G(k, \tau)$. Going back to equation (1.13) and transforming the creation and annihilation operators to the pseudo-interaction picture described in Appendix B yields
\[
G(k, \tau) = -\frac{1}{\hbar} tr \left( \frac{e^{-\beta K} T_\tau \{e^{\tau K/h} e^{-\tau (H_0 - \mu N)/\hbar} c_{I k}(\tau) e^{\tau (H_0 - \mu N)/\hbar} e^{-\tau K/h} c_{I k}^\dagger(\tau) \}}{tr (e^{-\beta K})} \right)
\]
\[
= -\frac{1}{\hbar} tr \left( \frac{e^{-\beta (H_0 - \mu N)} e^{\beta (H_0 - \mu N)} e^{-\beta K} T_\tau \{S(0, \tau) c_{I k}(\tau) S(\tau, 0) c_{I k}^\dagger(\tau) \}}{tr (e^{-\beta (H_0 - \mu N)} e^{\beta (H_0 - \mu N)} e^{-\beta K})} \right)
\]
\[
= -\frac{1}{\hbar} tr \left( \frac{e^{-\beta K_0} T_\tau \{S(h \beta, 0) c_{I k}(\tau) S(\tau, 0) c_{I k}^\dagger(\tau) \}}{tr (e^{-\beta K_0} S(h \beta, 0))} \right)
\]
\[
= -\frac{1}{\hbar} tr \left( \frac{e^{-\beta K_0} T_\tau \{S(h \beta, 0) c_{I k}(\tau) c_{I k}^\dagger(\tau) \}}{tr (e^{-\beta K_0} S(h \beta, 0))} \right) = -\frac{1}{\hbar} \langle T_\tau \{S(h \beta, 0) c_{I k}(\tau) c_{I k}^\dagger(\tau) \} \rangle_0.
\] (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 $\rho_0$ and $S$, $c_{I k}$ and $c_{I k}^\dagger$ 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 $G(k, \tau)$. This must be taken into account for the Feynman diagrams.
1.3 Equilibrium Finite Temperature Green’s Functions

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)

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

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

(1.19)

where the brackets $\langle \cdots \rangle$ 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 $G^R$

$$G^R(k, t) = -\frac{i}{\hbar} \theta(t) \langle [c_k(t), c_k^\dagger]_+ \rangle$$

$$= -\frac{i}{\hbar} \theta(t) \frac{\text{tr} \left( e^{-\beta K \hat{K}} c_k e^{-it \hat{K}/\hbar} c_k^\dagger \right) \left( e^{-\beta K} \right)}{\text{tr} \left( e^{-\beta K} \right)}$$

$$= -\frac{i}{\hbar} \theta(t) \sum_{nm} \frac{\langle n | e^{-\beta K} e^{it \hat{K}/\hbar} c_k e^{-it \hat{K}/\hbar} | m \rangle \langle m | c_k^\dagger | n \rangle}{\text{tr} \left( e^{-\beta K} \right)}$$

$$= -\frac{i}{\hbar} \theta(t) \sum_{nm} \frac{e^{-it(K_n - K_m) / \hbar} \langle n | c_k | m \rangle^2 \left( e^{-\beta K_n} + e^{-\beta K_m} \right)}{\text{tr} \left( e^{-\beta K} \right)}$$

(1.20)

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

$$G^R(k, \omega) = \frac{1}{\text{tr} \left( e^{-\beta K} \right)} \sum_{nm} \frac{|\langle n | c_k | m \rangle|^2 \left( e^{-\beta K_m} + e^{-\beta K_n} \right)}{\hbar \omega + K_n - K_m + i\delta}$$

$$= [G^A(k, \omega)]^\dagger.$$

(1.21)

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

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

(1.22)

Therefore, with knowledge of the Matsubara Green’s function $G$, for which a perturbation expansion can easily be derived, a real-time Green’s function $G^R$ can be found.

$$G^R(k, \omega) = G(k, i\omega_n \to \omega + i\delta)$$

(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

\[
G^<(x,t; x', t') = \frac{i}{\hbar} \langle \hat{\psi}^\dagger (x', t') \hat{\psi} (x,t) \rangle
\]

\[
G^>(x,t; x', t') = -\frac{i}{\hbar} \langle \hat{\psi} (x, t) \hat{\psi}^\dagger (x', t') \rangle
\]

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]

\[
G(x,t; x', t') = \theta(t - t')G^>(x,t; x', t') + \theta(t' - t)G^<(x,t; x', t')
\]

(1.25)

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

(1.26)

\[
G^R(x,t; x', t') - G^A(x,t; x', t') = G^>(x,t; x', t') - G^<(x,t; x', t').
\]

(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

\[
A(k, \omega) = i(G^R(k, \omega) - G^A(k, \omega)) = i(G^>(k, \omega) - G^<(k, \omega))
\]

(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

\[
G^>(\omega) = -e^{\beta(\hbar \omega - \mu)}G^<(\omega)
\]

(1.29)

and for the spectral function

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

(1.30)

or

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

(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

\[
n(x) = -i\hbar G^<(x, t; x, t)
\]

(1.32)
and for an homogeneous system

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

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

\[
Z(\omega) = \frac{1}{V} \sum_k \frac{A(k,\omega)}{2\pi} = \frac{i\hbar}{2\pi} \sum_k \frac{G^R(k,\omega) - G^A(k,\omega)}{2\pi} \tag{1.34}
\]

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

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

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

\[
G^R_0(k,\omega) = \frac{1}{\hbar \omega - E_k + i\delta} \quad \text{and} \quad G^A_0(k,\omega) = \frac{1}{\hbar \omega - E_k - i\delta} \tag{1.36}
\]

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

\[
A(k,\omega) = 2\pi \delta(\omega - E_k/\hbar) \tag{1.37}
\]

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 \( \delta \) 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 \( G^< \)

\[
j(x,t) = \frac{\hbar^2}{2m} \lim_{x' \to x} (\nabla' - \nabla) G^<(x,t;x',t). \tag{1.38}
\]

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 $t_0$ instead of 0 as in Appendix A, and then transforms it into the interaction representation, one has

$$
\langle O_H(t) \rangle = \langle S(t_0, t) O_I(t) S(t, t_0) \rangle
$$

$$
= \langle T^a \left\{ \exp \left( \frac{i}{\hbar} \int_{t_0}^{t} dt' V_I(t') \right) \right\} O_I(t) T^c \left\{ \exp \left( -\frac{i}{\hbar} \int_{t_0}^{t} dt' V_I(t') \right) \right\} \rangle
$$

\hspace{1cm} (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

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

\hspace{1cm} (1.40)

where $\oint_{C}$ 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 $t_0$. 
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,

$$G(x,t;x',t') = -\frac{i}{\hbar} \langle T \{ \hat{\psi}_H(x,t)\hat{\psi}_H^\dagger(x',t') \} \rangle$$  \hspace{1cm} (1.41)

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

$$G(x,t;x',t') = \theta(t,t')G^>(x,t;x',t') + \theta(t',t)G^<(x,t;x',t')$$ \hspace{1cm} (1.42)

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

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

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

$$\mathcal{H}(t) = H + H^{\text{ext}}(t) = H_0 + V + H^{\text{ext}}(t),$$ \hspace{1cm} (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 $H^{\text{ext}}(t)$ is an external perturbation driving the system out of equilibrium

$$H^{\text{ext}}(t) = \int dx \, \hat{\psi}^\dagger(x)U(x,t)\hat{\psi}(x)$$ \hspace{1cm} (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]

$$G(x,t;x',t') = -\frac{i}{\hbar} \langle \sqrt{T} \{ S^{\text{ext}}_{H}(t_0,t_0)\hat{\psi}_H(x,t)\hat{\psi}_H^\dagger(x',t') \} \rangle$$ \hspace{1cm} (1.46)

where the term $S^{\text{ext}}_{H}(t_0,t_0)$ with

$$S^{\text{ext}}_{H}(t_0,t_0) = T \left\{ \exp \left( -\frac{i}{\hbar} \int_C \! dt \, H^{\text{ext}}_{H}(t) \right) \right\},$$ \hspace{1cm} (1.47)

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

$$\langle \cdots \rangle = \frac{\text{tr}(\rho(t_0)\cdots)}{\text{tr}(\rho(t_0))} = \frac{\text{tr}(e^{-H_{\text{initial}}(\cdots)}}{\text{tr}(e^{-H_{\text{initial}}})}.$$ \hspace{1cm} (1.48)

$H_{\text{initial}} = H_0 + V$ 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 $H_{\text{initial}} = \mathcal{H}_0$ 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

$$
G(x, t; x', t') = -\frac{i}{\hbar} \frac{\langle [S^{ext}_{\mathcal{H}_0}(t_0, t_0)S^V_{\mathcal{H}_0}(t_0, t_0)\hat{\psi}_{\mathcal{H}_0}(x, t)\hat{\psi}_{\mathcal{H}_0}(x', t')]_0 \rangle}{\langle S^{ext}_{\mathcal{H}_0}(t_0, t_0)S^V_{\mathcal{H}_0}(t_0, t_0) \rangle_0}
$$

(1.49)

where $t_0 = -\infty$ and

$$
S^{ext}_{\mathcal{H}_0}(t_0, t_0) = T \left\{ \exp \left( -\frac{i}{\hbar} \int_C dt H^{ext}_{\mathcal{H}_0}(t) \right) \right\}
$$

$$
S^V_{\mathcal{H}_0}(t_0, t_0) = T \left\{ \exp \left( -\frac{i}{\hbar} \int_C dt V_{\mathcal{H}_0}(t) \right) \right\}.
$$

(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. $H^{xt}(t)$ will be included through the time evolution operator $S_{H}^{xt}(t, t_0)$ of equation (1.46). $H$ contains only the carrier-carrier interactions here, carrier-phonon scattering will be treated in Appendix F. This yields for $H$

\[
H = H_0 + V = \int dx \, \hat{\psi}^\dagger(x) \left(-\frac{\hbar^2 \nabla^2}{2m}\right) \hat{\psi}(x) + \frac{1}{2} \int dx \int dy \, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) V(x-y) \hat{\psi}(y) \hat{\psi}(x). \quad (2.1)
\]

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: \(1 = (x_1, t_1), V(1 - 2) = V(x_1 - x_2)\delta(t_1 - t_2), \oint_C \mathrm{d}t = \oint_C \mathrm{d}t_1 \int \mathrm{d}x_1,\)

where the time is integrated along a contour \(C\) such as the one of Figure 1.1,

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

and \(\delta(1') = \delta(t_1, t_1')\delta(x_1 - x_1').\) Furthermore, the following equation has to be evaluated in order to obtain \(\frac{\mathrm{d}}{\mathrm{d}t}G(x, t; x', t'):\)

\[
\frac{\mathrm{d}}{\mathrm{d}t} T \left\{ \psi_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\} = T \left\{ \frac{\mathrm{d}}{\mathrm{d}t} \psi_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\} + \delta(t, t') \left[ \psi_H(x, t) \hat{\psi}_H^\dagger(x', t) \right] + \delta(t, t')\delta(x - x'),
\]

to take into account the time-ordering operator \(T,\)

\[
i\hbar T \left\{ \frac{\mathrm{d}}{\mathrm{d}t} \left( S^\text{ext}_H(t_0, t_0) \psi_H(x, t) \hat{\psi}_H^\dagger(x', t') \right) \right\} = i\hbar T \left\{ \frac{\mathrm{d}}{\mathrm{d}t} \left( S^\text{ext}_H(t_0, t) \psi_H(x, t) S^\text{ext}_H(t, t_0) \cdots \right) \right\}
\]

\[
= T \left\{ S^\text{ext}_H(t_0, t_0)i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \psi_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\}
\]

\[
+ T \left\{ S^\text{ext}_H(t_0, t_0)U(x, t) \psi_H(x, t) \hat{\psi}_H^\dagger(x', t') \right\},
\]

to look after the time evolution \(S^\text{ext}_H,\) and

\[
i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \hat{\psi}_H(x, t) = \left[ \hat{\psi}_H(x, t), H_H(t) \right]
\]

\[
= -\frac{\hbar^2 \nabla^2}{2m} \hat{\psi}_H(x, t) + \int \mathrm{d}y \, V(x - y) \hat{\psi}_H^\dagger(y, t) \hat{\psi}_H(y, t) \hat{\psi}_H(x, t)
\]

for the operator derivative (Heisenberg equation of motion).

### 2.2.1 Dyson Equations

With the previous considerations, the equation of motion for \(G(x_1, t_1; x_1', t_1') = G(1')\) relative to \(t_1\) becomes

\[
\left( i\hbar \frac{\mathrm{d}}{\mathrm{d}t_1} + \frac{\hbar^2 \nabla^2}{2m} - U(1) \right) G(1') = \delta(1') - i\hbar \int_C \mathrm{d}3 \, V(1 - 3) \, G^{(2)}(13^-1'3^+)
\]

(2.2)

and relative to \(t_1'\)

\[
\left( -i\hbar \frac{\mathrm{d}}{\mathrm{d}t_1'} + \frac{\hbar^2 \nabla^2}{2m} - U(1') \right) G(1') = \delta(1') - i\hbar \int_C \mathrm{d}3 \, V(1' - 3) \, G^{(2)}(13^-1'3^+)
\]

(2.3)
where the 2-particle Green’s function $G^{(2)}(131'3')$ is defined by

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

The self-energy $\Sigma^{\text{tot}}(12)$ 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

$$\left( i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla^2_1}{2m} - U(1) \right) G(11') = \delta(11') + \int_C d3 \Sigma^{\text{tot}}(13) G(31') \tag{2.5}$$

$$\left( -i\hbar \frac{d}{dt_1'} + \frac{\hbar^2 \nabla^2_{1'}}{2m} - U(1') \right) G(11') = \delta(11') + \int_C d3 G(13) \Sigma^{\text{tot}}(31'). \tag{2.6}$$

They correspond to the Dyson equations

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

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

where $G_0(12)$ is the free or non-interacting nonequilibrium Green’s function and $G^{-1}_0(12)$ its inverse, defined by

$$G_0(12) = \left( i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla^2_1}{2m} - U(1) \right)^{-1} \delta(12) \tag{2.9}$$

$$G^{-1}_0(12) = \left( i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla^2_{1'}}{2m} - U(1') \right) \delta(12). \tag{2.10}$$

This gives the following relations

$$\int_C d2 G^{-1}_0(12) G_0(21') = \delta(11') \tag{2.11}$$

$$\int_C d2 G^{-1}_0(12) G(21') = \left( i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla^2_{1'}}{2m} - U(1') \right) G(11'). \tag{2.12}$$

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,

\[
C(t_1, t'_1) = \int_{C_1} d\tau \ A(t_1, \tau) B(\tau, t'_1), \tag{2.13}
\]

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)

\[
C(t_1, t'_1) = \theta(t_1, t'_1) C^>(t_1, t'_1) + \theta(t'_1, t_1) C^<(t_1, t'_1), \tag{2.14}
\]

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

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

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

\[
\int_{C_2} d\tau \ A(t_1, \tau) B^<(\tau, t'_1) = \int_{-\infty}^{t_1} dt \ A^>(t_1, t) B^<(\tau, t'_1) + \int_{t_1}^{-\infty} dt \ A^<(t_1, t) B^<(\tau, t'_1)
\]

\[
= \int_{-\infty}^{t_1} dt \ (A^>(t_1, t) - A^<(t_1, t)) B^<(\tau, t'_1)
\]

\[
= \int_{-\infty}^{t_1} dt \ A^R(t_1, t) B^<(\tau, t'_1). \tag{2.16}
\]
In the first line, \( A(t_1, t) \) is equal to \( A^\tau(t_1, t) \) 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

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

and therefore in compact notation \( C^< = A^R B^< + A^< B^A \). 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 \( C^R (t_1, t'_1) \)

\[
C^R (t_1, t'_1) = \theta(t_1 - t'_1) \left( C^> (t_1, t'_1) - C^< (t_1, t'_1) \right)
\]

\[
= \theta(t_1 - t'_1) \int_{-\infty}^{\infty} dt \left( A^R [B^> - B^<] + [A^> - A^<] B^A \right)
\]

\[
= \theta(t_1 - t'_1) \left[ \int_{-\infty}^{t_1} dt (A^> - A^<)(B^> - B^<) + \int_{-\infty}^{t'_1} dt (A^> - A^<)(B^< - B^>) \right]
\]

\[
= \int_{t'_1}^{t_1} dt (A^> - A^<)(B^> - B^<)
\]

\[
= \int_{t'_1}^{t_1} dt A^R(t_1, t)B^R(t, t'_1). \tag{2.18}
\]

In the compact form, this relation is expressed as \( C^R = A^R B^R \) 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

\[
D(t_1, t'_1) = \int_{C_1} d\tau_1 \int_{C_1} d\tau_2 A(t_1, \tau_1)B(\tau_1, \tau_2)C(\tau_2, t'_1)
\]

\[
= \int_{C_1} d\tau_1 A(t_1, \tau_1)B'(\tau_1, t'_1) \tag{2.19}
\]

and

\[
B'(\tau_1, t'_1) = \int_{C_1} d\tau_2 B(\tau_1, \tau_2)C(\tau_2, t'_1). \tag{2.20}
\]

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

\[
D^< = A^R B^R C^< + A^R B^< C^A + A^< B^A C^A. \tag{2.21}
\]
Other structures are of great interest in order to evaluate the self energies
\[ C(t, t') = A(t, t')B(t, t') \]
\[ D(t, t') = A(t, t')B(t', t) \]
where \( t \) and \( t' \) are contour variables. It is obvious that
\[ C^<(t, t') = A^<(t, t')B^<(t, t') \]
\[ D^<(t, t') = A^<(t, t')B^>(t', t) \]
and a little more complicated for \( C^R, C^A, D^R \) and \( D^A \)
\[ C^R(t, t') = \theta(t - t') (C^>(t, t') - C^<(t, t')) \]
\[ = \theta(t - t') (A^>(t, t')B^>(t, t') - A^<(t, t')B^<(t, t')) \]
\[ = \theta(t - t') (A^>(t, t')B^>(t, t') - A^<(t, t')B^>(t, t') + A^<(t, t')B^>(t, t') - A^<(t, t')B^<(t, t')) \]
\[ C^A(t, t') = A^A(t, t')B^A(t, t') + A^A(t, t')B^>(t, t') + A^>(t, t')B^<(t, t') + A^>(t, t')B^A(t, t') \]
\[ = -A^A(t, t')B^A(t, t') + A^A(t, t')B^>(t, t') + A^>(t, t')B^A(t, t') \]
\[ D^R(t, t') = A^R(t, t')B^>(t, t') + A^<(t, t')B^>(t, t') + A^<(t, t')B^>(t, t') \]
\[ D^A(t, t') = A^A(t, t')B^>(t, t') + A^<(t, t')B^>(t, t') \]
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 \( r \) and \( r' \). 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]
\[ G(11') = \sum_{n_1, m_1} \sum_{k', k''} \phi_{n_1, k'}(r) \cdot G_{n_1 m_1}(k' k'; tt') \cdot \phi^*_{m_1, k''}(r'). \]  
(2.23)

For homogeneity in the \( x \)- and \( y \)- directions and confinement in the \( z \)-one, one can factorize the wave functions \( \phi \) as
\[ \phi_k(r) = \frac{1}{\sqrt{A}} e^{ikx} \phi_{k\ell}(z), \]  
(2.24)
where $A$ is the xy surface, $k_t = (k_x, k_y)$, and $r_t = (x, y)$. Furthermore, because of
the homogeneity in the $x-$ and $y-$ directions, the Green’s function $G(11')$ depends
only on the difference $r_t - r'_t$ and, therefore, $k'_t = k'_t$. This gives

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

The wave functions $\phi$ should be very localized functions, for example orbital func-
tions 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

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

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

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

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

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

$$i\hbar \frac{d}{dt} G_{nm}(k_t; tt') - \sum_{l} h_{nl} G_{lm}(k_t; tt') = \delta_{nm}(tt') + \sum_{l} \int dt_1 \Sigma_{nl}(k_t; tt_1) G_{lm}(k_t; tt_1)$$

and

$$-i\hbar \frac{d}{dt} G_{nm}(k_t; tt') - \sum_{l} h^{*}_{nl} G_{nl}(k_t; tt') = \delta_{nm}(tt') + \sum_{l} \int dt_1 G_{nl}(k_t; tt_1) \Sigma_{lm}(k_t; tt_1)$$

where $h_{nm} = \int \text{d}r \phi^{*}_{n}(r) H_0(r) \phi_{m}(r)$ and $h^{*}_{nl} = h_{nl}$, because the Hamiltonian is
hermitian.

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

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

With the help of equation (2.28), one gets

$$\Sigma_{nm}(k_t; tt') = i\hbar \int d(r_t - r'_t) \int dz \int dz' \phi^{*}_{n,k_t}(z) \cdot W(11') \cdot G(11') \cdot \phi_{m,k_t}(z') \cdot e^{-ik'_t(r_t - r'_t)}.$$
Expanding $G(11')$ in this equation yields

$$
\Sigma_{nm}(k'|tt') = \frac{i}{\hbar} \sum_{n,m_1} \sum_{k'_t} \int d(r_t - r'_t) \int dz' G_{n,m_1}(k'_t;tt')
$$

$$
\times \phi^*_{n,k_t}(z) \phi_{m,k_t}(z') \cdot W(1'1) \cdot \phi^*_{m_1,k'_t}(z') e^{-i(k'_t-k_t) \cdot (r'_t-r_t)}
$$

$$
= \frac{i}{\hbar} \sum_{n_1,m_1} \sum_{k'_t} W_{n_1,m_1}(k'_t - k_t; t't) G_{n_1,m_1}(k'_t; tt').
$$

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 $G^<(x, x'; t, t')$, 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

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

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

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

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

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

$$
i \hbar \frac{d}{dt} G_{nm}(k_t; tt') - \sum_l h_{nl} G^<_{lm}(k_t; tt') = \sum_l \int_{t_0}^\infty dt_1 \Sigma^R_{nl}(k_t; tt_1) G^<_{lm}(k_t; tt_1)
$$

$$
+ \sum_l \int_{t_0}^\infty dt_1 \Sigma^<_{nl}(k_t; tt_1) G^A_{lm}(k_t; tt_1)
$$

(2.34)
and/or
\[-i\hbar \frac{d}{dt} G_{nm}^\lt(k_t; tt') - \sum_l G_{nl}(k_t; tt') h_{lm} = \sum_l \int_{t_0}^\infty dt_1 G_{nl}^R(k_t; tt_1) \Sigma_n^\lt(k_t; t_1 t') + \sum_l \int_{t_0}^\infty dt_1 G_{nl}^\lt(k_t; tt_1) \Sigma_n^A(k_t; t_1 t'). \tag{2.35}\]

To solve one of these equations, one needs different forms of the self-energy ($\Sigma^\lt$ 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
\[i\hbar \frac{d}{dt} G_{nm}^R(k_t; tt') - \sum_l h_{nl} G_{lm}^R(k_t; tt') = \delta_{nm}(tt') + \sum_l \int_{t_0}^\infty dt_1 \Sigma_n^R(k_t; tt_1) G_{lm}^R(k_t; t_1 t') \]

or
\[-i\hbar \frac{d}{dt} G_{nm}^R(k_t; tt') - \sum_l G_{nl}^R(k_t; tt') h_{lm} = \delta_{nm}(tt') + \sum_l \int_{t_0}^\infty dt_1 G_{nl}^R(k_t; tt_1) \Sigma_n^R(k_t; t_1 t'). \]

The equations for $G^A$ are obtained by replacing the $R$’s by $A$’s. One can rewrite them in a compact form
\[\delta_{nm}(tt') = \sum_l \int_{t_0}^\infty dt_1 \left( i \hbar \delta_{lm}(t_1 t) \frac{d}{dt_1} - h_{nl} \delta(t_1 t) - \Sigma_n^R(k_t; tt_1) \right) G_{lm}^R(k_t; t_1 t') \]

\[= \sum_l \int_{t_0}^\infty dt_1 \left[ G_{nl}^R(k_t; tt_1) \right]^{-1} G_{lm}^R(k_t; t_1 t'). \tag{2.36}\]

Relation 2.36 can be used to simplify the equation of motion for the lesser Green’s function $G^\lt$
\[\sum_l \int_{t_0}^\infty dt_1 \left[ G_{nl}^R(k_t; t_1 t') \right]^{-1} G_{lm}^\lt(k_t; t_1 t'') = \sum_l \int_{t_0}^\infty dt_1 \Sigma_n^\lt(k_t; t_1 t') G_{lm}^A(k_t; t_1 t''). \]

Multiplying each side of the equation by $G_{pm}^R(k_t; tt')$, summing over $n$, and integrating over $t'$ yields
\[\sum_{l,n} \int_{t_0}^\infty dt_1 \int_{t_0}^\infty dt' G_{pm}^R(k_t; tt') \left[ G_{nl}^R(k_t; t_1 t') \right]^{-1} G_{lm}^\lt(k_t; t_1 t'') = \sum_l \int_{t_0}^\infty dt_1 \delta_{pl}(tt_1) G_{lm}^\lt(k_t; t_1 t'') = G_{pm}^\lt(k_t; tt''). \]

and therefore
\[G_{nm}^\lt(k_t; tt') = \sum_{l,v} \int_{t_0}^\infty dt_1 \int_{t_0}^\infty dt_2 G_{nl}^R(k_t; tt_1) \Sigma_{lv}^\lt(k_t; t_1 t_2) G_{vm}^A(k_t; t_2 t'). \tag{2.37}\]

This is the central equation for the lesser Green’s function, but there is still a coupling between $G^\lt$ and $G^{R,A}$.
and the inverse Fourier transformation of the equations

\[ G_{0nm}^{\lesssim}(k; t_1 t_2) = \frac{i}{\hbar} \langle \hat{c}_{k,m}^\dagger(t_2) c_{k,n}(t_1) \rangle, \]  

(2.38)

where the creation \( \hat{c}_{k,m}^\dagger(t) \) and annihilation \( c_k(t) \) operators are defined with respect to the non-interacting Hamiltonian \( H_0 \)

\[ c_k^\dagger(t) = e^{iH_0 t/\hbar} c_k^\dagger e^{-iH_0 t/\hbar}, \]
\[ c_k(t) = e^{iH_0 t/\hbar} c_k e^{-iH_0 t/\hbar}. \]  

(2.39)

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

\[ G_{0nm}^{\lesssim}(k; t_1 t_2) = \frac{i}{\hbar} e^{iE_{m1}/\hbar} e^{-iE_{n1}/\hbar} \langle \hat{c}_{k,m}^\dagger c_{k,n} \rangle. \]  

(2.40)

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

\[ G_{0nm}^{\gtrsim}(k; t_1 t_2) = -\frac{i}{\hbar} e^{iE_{m1}/\hbar} e^{-iE_{n1}/\hbar} \langle \hat{c}_{k,m}^\dagger c_{k,n} \rangle. \]  

(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 \( G^A \)

\[ G_{0nm}^{R}(k; t_1 t_2) = \theta(t_1 - t_2) (G_{0nm}^{\gtrsim}(k; t_1 t_2) - G_{0nm}^{\lesssim}(k; t_1 t_2)) \]
\[ = -\frac{i}{\hbar} \theta(t_1 - t_2) e^{iE_{m1}/\hbar} e^{-iE_{n1}/\hbar} \langle [\hat{c}_{k,n}, \hat{c}_{k,m}^\dagger] \rangle \]
\[ = -\frac{i}{\hbar} \theta(t_1 - t_2) e^{iE_{m1}/\hbar} e^{-iE_{n1}/\hbar} \delta_{nm}, \]
\[ G_{0nm}^{A}(k; t_1 t_2) = \frac{i}{\hbar} \theta(t_2 - t_1) e^{iE_{m1}/\hbar} e^{-iE_{n1}/\hbar} \delta_{nm}. \]  

(2.42)

### 2.5.2 Stationary Solution

Once the stationary solution of a nonequilibrium system is reached, the Green’s functions \( G_{nm}(k_1; t t') \) 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

\[ G_{nm}^{\lesssim}(k_1; E) = \int dt (t - t') e^{iE(t-t')/\hbar} G_{nm}^{\lesssim}(k_1; t - t') \]  

(2.43)

and the inverse Fourier transformation

\[ G_{nm}^{\lesssim}(k_1; t - t') = \frac{1}{2\pi\hbar} \int dE e^{-iE(t-t')/\hbar} G_{nm}^{\lesssim}(k_1; E). \]  

(2.44)
The same relations hold for $G^{R,A}$. This produces simplified equations of motion for the stationary state of the system

\[
EG^{<}_{nm}(k_t; E) - \sum_l h_{nl} G^{<}_{lm}(k_t; E) = \sum_l \Sigma^{R}_{nl}(k_t; E) G^{<}_{lm}(k_t; E) + \sum_l \Sigma^{<}_{nl}(k_t; E) G^{A}_{lm}(k_t; E)
\]

\[
EG^{<}_{nm}(k_t; E) - \sum_l G^{<}_{nl}(k_t; E) h_{lm} = \sum_l G^{R}_{nl}(k_t; E) \Sigma^{<}_{lm}(k_t; E) + \sum_l G^{<}_{nl}(k_t; E) \Sigma^{A}_{lm}(k_t; E)
\]

\[
G^{<}_{nm}(k_t; E) = \sum_{l,v} G^{R}_{nl}(k_t; E) \Sigma^{<}_{vl}(k_t; E) G^{A}_{vm}(k_t; E)
\]

\[
G^{<}_{nm}(k_t; E) = -[G^{<}_{nm}(k_t; E)]^\dagger
\]

\[
EG^{R}_{nm}(k_t; E) - \sum_l h_{nl} G^{R}_{lm}(k_t; E) = \delta_{nm} + \sum_l \Sigma^{R}_{nl}(k_t; E) G^{R}_{lm}(k_t; E)
\]

\[
G^{A}_{nm}(k_t; E) = [G^{R}_{nm}(k_t; E)]^\dagger
\]

\[
G^{R}_{nm}(k_t; E) - G^{A}_{nm}(k_t; E) = G^{<}_{nm}(k_t; E) - G^{<}_{nm}(k_t; E)
\]

\[
A(k_t; E) = i (G^{R}_{nm}(k_t; E) - G^{A}_{nm}(k_t; E))
\]

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 $\Sigma^{<}_{nm}(k_t; E)$ and $\Sigma^{R}_{nm}(k_t; E)$ 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 $G^{R}$, $G^{<}$, $\Sigma^{R}$, 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 $\Sigma^{R}$ 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 $\Sigma^{R}$ 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 $G^{<}$.
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.

<table>
<thead>
<tr>
<th>$\Sigma^{\text{Hartree}}(12)$</th>
<th>$\Sigma^{\text{Fock}}(12)$</th>
<th>$\Sigma^{\text{dc}}(12)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-i\hbar \delta(12) \int d^3 V(1-3)G(33^+)$</td>
<td>$i\hbar V(1-2)G(12)$</td>
<td>$i\hbar \int d^3 \int d^4 V(2-3)\pi(34)W(41)G(12)$</td>
</tr>
</tbody>
</table>

with

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

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

$$ U_{\text{eff}}(1) = U(1) - i\hbar \int d^2 V(1-2)G(22^+) $$
2.5 Closed Set of Equations

\[
U(1) + \int d^3r_2 V(r_1 - r_2)n(r_2 t)
\]

\[
= U(1) - \frac{1}{e} \int d^3r_2 \frac{e^2}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \rho(r_2 t), \quad n(r_2 t) = -\frac{1}{e}\rho(r_2 t)
\]

\[
= U(1) - e\phi(1),
\]

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

\[
\phi(1) = \int d^3r_2 \frac{1}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \rho(r_2 t)
\]

\[
E(1) = -\text{grad} \phi(1) = \int d^3r_2 \frac{r_1 - r_2}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \rho(r_2 t)
\]

\[
\int E(1) \cdot dA = \int d^3r_1 \text{ div} E(1) = \int d^3r_2 \int \frac{dA(r_1 - r_2)}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \rho(r_2 t)
\]

\[
= \int d^3r_2 \int dA (r_1 - r_2) \rho(r_2 t)
\]

\[
= \int d^3r_2 \int d\theta \int_0^{2\pi} d\phi |\mathbf{r}_1 - \mathbf{r}_2|^2 \sin(\theta) \frac{1}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \rho(r_2 t)
\]

\[
= \int d^3r_2 \frac{\rho(r_2 t)}{r}
\]

\[
\Rightarrow \text{div} E(1) = -\text{div} \phi(1) = \frac{\rho(1)}{\epsilon}.
\]

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 \(\Sigma^{\text{Fock}}(12) = \Sigma^{\text{Fock}}(12) + \Sigma^{\text{dc}}(12)\)

\[
\Sigma^{\text{FDC}}_{nm}(k; t_1 t_2) = \frac{\hbar}{i} \sum_{n_1 m_1} \sum_{q} W_{nmn_1m_1}(q; t_2 t_1) G_{n_1 m_1}(k + q; t_1 t_2)
\]

(2.50)

where the inclusion of equation (F.13) delivers

\[
W_{nmn_1m_1}(q; t_2 t_1) = V_{nmn_1m_1}(q; t_2 t_1) + \sum_{n_2 m_2 m_3 m_4} \sum_{k_1} \int dt_3 \int dt_4 V_{nmn_3m_4}(q; t_2 t_3)
\]

\[
\times \pi_{nmn_3m_4}(k_1, k_1 - q; t_3 t_4) W_{nmn_4m_3}(q; t_4 t_1),
\]

(2.51)

\[
V_{nmn_1m_1}(q; t_2 t_1) = \frac{1}{A} \int d(r_{xy1} - r_{xy2}) \int dz_1 \int dz_2 \phi_n^*(z_1) \phi_m^*(z_2)V(2 - 1)\phi_{n_1}(z_1)\phi_{m_1}^*(z_2)e^{-iq(r_{xy2} - r_{xy1})},
\]

\[
W_{nmn_1m_1}(q; t_2 t_1) = \frac{1}{A} \int d(r_{xy1} - r_{xy2}) \int dz_1 \int dz_2 \phi_n^*(z_1) \phi_m(z_2)W(21)\phi_{n_1}(z_1)\phi_{m_1}^*(z_2)e^{-iq(r_{xy2} - r_{xy1})},
\]
\[ \pi_{nmn44m4}(k_1, k_1 - q; t_3 t_4) = -i h G_{nmn3}(k_1; t_3 t_4) G_{n44m4}(k_1 - q; t_4 t_3), \quad (2.52) \]

\[ q = (q_x, q_y), \text{ and } k_1 = (k_{1x}, k_{1y}). \] For the Fock self-energy only, one has

\[
\Sigma^{R\text{Fock}}_{nmn}(k; t_1 t_2) = \delta(t_1 - t_2) i \hbar \sum_{n_1 m_1} \sum_q V_{nmn1m_1}(q) G_{n1m_1}(k + q; t_1^+ t_2^+) \nonumber
\]

\[
= \delta(t_1 - t_2) i \hbar \sum_{n_1 m_1} \sum_q V_{nmn1m_1}(q) G_{n1m_1}^<(k + q; t_1 t_2). \nonumber
\]

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

\[
\Sigma_{nmn}^{d\langle}(k; t_1 t_2) = i \hbar \sum_{n_1 m_1} \sum_q W_{nmn1m_1}^{d\geq}(q; t_2 t_1) G_{n1m_1}^{<}(k + q; t_1 t_2). \quad (2.53)
\]

\[ \Sigma_{nmn}^{d\geq}(k; t_1 t_2) \] is calculated by inverting \(<\text{ and } >\). It remains to determine \(W_{nmn1m_1}^{d\geq}\).

From equation (2.51), one finds by neglecting the indices

\[
W^{d\geq}(t_2 t_1) = \int dt_3 \int dt_4 V(t_2 t_3) \pi^R(t_3 t_4) W^{d\geq}(t_4 t_1) + \int dt_3 \int dt_4 V(t_2 t_3) \pi^{d\geq}(t_3 t_4) W^A(t_4 t_1).
\]

This implies that

\[
\left[ \int dt_4 \left( \delta(t_4) - \int dt_3 V(t_2 t_3) \pi^R(t_3 t_4) \right) W^{d\geq}(t_4 t_1) \right] = \int dt_3 \int dt_4 V(t_2 t_3) \pi^{d\geq}(t_3 t_4) W^A(t_4 t_1),
\]

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

\[
\int dt_2 \int dt_4 \left[ \pi^R(t_2 t_4) \right]^{-1} \epsilon_R(t_2 t_4) W^{d\geq}(t_4 t_1) = \int dt_3 \int dt_4 \int dt_2 \left[ \epsilon_R(t_2 t_4) \right]^{-1} V(t_2 t_3) \pi^{d\geq}(t_3 t_4) W^A(t_4 t_1)
\]

and the final result

\[
W^{d\geq}_{nmn1m_1}(q; t_2 t_1) = \sum_{n_3 m_3 m_4} \sum_{k_1} \int dt_3 \int dt_4 W^R_{m_4 m_3 n_3 m_1}(q; t_2 t_3) \pi^{d\geq}_{n_3 m_3 m_4 n_4 m_1}(k_1; k_1 - q; t_3 t_4) W^A_{m_4 n_1 m_3}(q; t_4 t_1).
\]

The procedure to get \(W^{R,A}\) and \(\pi^{d\geq}\) is similar to the one needed for \(W^{d\geq}\) 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

\[
\Sigma_{nmn}^{d\geq}(k; E) = i \int \frac{dE'}{2\pi} \sum_{n_1 m_1} \sum_q W^{d\geq}_{nmn1m_1}(q; E') G_{n1m_1}^{<}(k + q; E - E'). \quad (2.54)
\]

The energy-dependent screened interaction \(W^{d\geq}(E')\) is given by

\[
W^{d\geq}_{nmn1m_1}(q; E') = \sum_{n_3 m_3 m_4} \sum_{k_1} W^R_{m_4 m_3 n_3 m_1}(q; E') \pi^{d\geq}_{n_3 m_3 m_4}(k_1, k_1 - q; E') W^A_{m_4 n_1 m_3}(q; E')
\]
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with

\[ \pi^>_n(k_1, k_1 - q; E') = -i \int \frac{dE''}{2\pi} G^>_n(k_1; E'')G^<_n(k_1 - q; E'' - E') \]

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

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

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))

\[ H^{FR} = \int dr \hat{\psi}^\dagger(r) \sum_q \frac{\epsilon_{qr}}{|q|} (C a_q + C^* a_{-q}^\dagger) \hat{\psi}(r) \]

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

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

\( C \) 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))

\[ \Sigma^{ph}(12) = i\hbar |C|^2 \sum_{q_1,q_2} \frac{\epsilon_{q_1 q_2}}{|q_1| |q_2|} D(q_1 q_2; t_1 t_2) G(12) \]

with, derived from equation (F.62),

\[ D(q_1 q_1; t_1 t_2) = -i \frac{1}{\hbar} \langle T \{ S[a_{q_1}(t_1) a_{-q_2}^\dagger(t_2) + a_{-q_1}^\dagger(t_1) a_{q_2}(t_2) \} \rangle \delta_{q_1, -q_2} \]

The eigenfunction expansion of (2.58) yields

\[ \Sigma^{ph}_{nm}(k; t_1 t_2) = i\hbar \sum_{m_1 m_1} \sum_q M_{n m_1}(q) M^*_{m_1 m_1}(q) D(q; t_1 t_2) G_{n m_1}(k - q; t_1 t_2) \]

where the form factor \( M_{n m_1}(q) \) and \( D(q; t_1 t_2) \) are

\[ M_{n m_1}(q) = \left| \frac{C}{q} \right| \int dz \phi_n^*(z) e^{iqz} \phi_{m_1}(z) \] and \( D(q; t_1 t_2) = D(q, -q; t_1 t_2) \).
To find the lesser and the retarded self-energies, Langreth theorem from section 2.3 is applied

\[
\Sigma_{nn}^{< (R)}(k; t_1 t_2) = \begin{cases} 
\frac{i \hbar}{2 \mathcal{P}} \sum_{n1m1} \int \frac{dE'}{2\pi} M_{nn_1}(q) M_{m1n_1}^{*}(q) D^{<}(q; t_1 t_2) G^{<}_{n1m1}(k - q_l| t_1 t_2) \\
+ i \hbar \sum_{q} M_{nn_1}(q) M_{m1n_1}^{*}(q) \left\{ D^{R}(q; t_1 t_2) G^{R}_{n1m1}(k - q_l| t_1 t_2) + D^{<}(q; t_1 t_2) G^{<}_{n1m1}(k - q_l| t_1 t_2) \right\} 
\end{cases}
\]

(2.61)

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

\[
\Sigma_{nn}^{< (R)}(k; E) = \begin{cases} 
i \hbar \sum_{n1m1} \sum_{q} \int \frac{dE'}{2\pi} M_{nn_1}(q) M_{m1n_1}^{*}(q) D^{<}(q; E') G^{<}_{n1m1}(k - q_l| E - E') \\
+ i \hbar \sum_{q} M_{nn_1}(q) M_{m1n_1}^{*}(q) \left\{ D^{R}(q; E') G^{R}_{n1m1}(k - q_l| E - E') + D^{<}(q; E') G^{<}_{n1m1}(k - q_l| E - E') \right\} 
\end{cases}
\]

(2.62)

For a complete set of equations Dyson’s equation for the phonon Green’s function \(D(q; E)\) 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 \(D^{(0)}(q; E)\) from equation (F.64) can replace \(D(q; E)\). Thus one will use the following expressions

\[D^{R}(q; E') = \frac{1}{E' - \hbar \omega_q + i \delta} - \frac{1}{E' + \hbar \omega_q + i \delta} \]

\[D^{<}(q; E') = -2\pi i \left[ N_q \delta(E' - \hbar \omega_q) + (N_q + 1) \delta(E' + \hbar \omega_q) \right]. \tag{2.63}\]

\(N_q\) is the Bose distribution for the phonons and \(\omega_q\) 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

\[
i \int \frac{dE'}{2\pi} D^{<}(E') G^{<}(E - E') = \int dE' G^{<}(E - E') \left[ N_q \delta(E' - \hbar \omega_q) + (N_q + 1) \delta(E' + \hbar \omega_q) \right]
\]

\[
= N_q G^{<}(E - \hbar \omega_q) + (N_q + 1) G^{<}(E + \hbar \omega_q)
\]

\[
i \int \frac{dE'}{2\pi} D^{<}(E') G^{R}(E - E') = N_q G^{R}(E - \hbar \omega_q) + (N_q + 1) G^{R}(E + \hbar \omega_q)
\]

\[
i \int \frac{dE'}{2\pi} D^{R}(E') G^{<}(E - E') = \frac{1}{2} \int dE' G^{<}(E - E') \left[ \delta(E' - \hbar \omega_q) - \delta(E' + \hbar \omega_q) \right]
\]
\[ \Sigma_{nm}^{\text{ph}}(k; E) = \sum_{n_1m_1} \sum_q M_{nm_1}(q) M^*_{m_1m}(q) \{ N_q G^<(k - q||; E - \hbar \omega_q) + (N_q + 1) G^<(k - q||; E + \hbar \omega_q) \} \]

\[ \Sigma_{nm}^{\text{Rph}}(k; E) = \sum_{n_1m_1} \sum_q M_{nm_1}(q) M^*_{m_1m}(q) [(N_q + 1) G^R(k - q||; E - \hbar \omega_q) + N_q G^R(k - q||; E + \hbar \omega_q) + \frac{1}{2} \left( G^<(k - q||; E - \hbar \omega_q) - G^<(k - q||; E + \hbar \omega_q) \right) + iP \left\{ \int \frac{dE'}{2\pi} \left( \frac{G^<(k - q||; E - E')}{E' - \hbar \omega_q} - \frac{G^<(k - q||; E + E')}{E' + \hbar \omega_q} \right) \right\}] \]

\[ \Sigma_{nm}^{\text{Aph}}(k; E) = \sum_{n_1m_1} \sum_q M_{nm_1}(q) M^*_{m_1m}(q) [(N_q + 1) G^A(k - q||; E - \hbar \omega_q) + N_q G^A(k - q||; E + \hbar \omega_q) + \frac{1}{2} \left( G^<(k - q||; E + \hbar \omega_q) - G^<(k - q||; E - \hbar \omega_q) \right) + iP \left\{ \int \frac{dE'}{2\pi} \left( \frac{G^<(k - q||; E - E')}{E' - \hbar \omega_q} - \frac{G^<(k - q||; E + E')}{E' + \hbar \omega_q} \right) \right\}] \]

The details for the advanced self-energy \( \Sigma_{nm}^{\text{Aph}}(k; E) \) are not given, but the procedure is the same as for \( \Sigma_{nm}^{\text{Rph}}(k; E) \), 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

\[ H^{\text{acph}} = \int dr \hat{\psi}^\dagger(r) \sum_q e^{iqr} |q| \left( U a_q + U^* a^\dagger_q \right) \hat{\psi}(r) \]  

(2.66)

where \( a_q \) and \( a^\dagger_q \) are the annihilation and creation phonon operators, respectively, and \( U = i \sqrt{\frac{\hbar D^2}{2\hbar m_e}} \). \( D \) is the material deformation potential, \( \rho \) 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 $M_{nn_1}(q)$

$$M_{nn_1}(q) = |U||q| \int dz \phi_n^*(z) e^{iqz} \phi_{n_1}(z) = |U||q|M'_{nn_1}(q)$$  \hspace{1cm} (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 $\omega_q$ is small. One has therefore

$$\omega_q = c_s |q|, \quad N_q = \frac{1}{e^{\hbar \omega_q/(k_B T)} - 1} \approx N_q + 1, \quad E' = \hbar \omega_q = E'.$$  \hspace{1cm} (2.68)

These assumptions lead to the following expressions

$$\Sigma_{nn_1}(k; E) = \frac{D^2 k_B T}{V \rho c_s} \sum_{n_1 m_1} \sum_q M'_{nn_1}(q) M_{mn_1}(q) G_{n_1 m_1}(k - |q|; E)$$

$$\Sigma_{nn_1}(k; E) = \frac{D^2 k_B T}{V \rho c_s} \sum_{n_1 m_1} \sum_q M'_{nn_1}(q) M_{mn_1}(q) G_{n_1 m_1}(k - |q|; E)$$ \hspace{1cm} (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

$$H^{is} = \sum_i \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) V(\mathbf{r} - \mathbf{R}_i) \hat{\psi}(\mathbf{r}),$$  \hspace{1cm} (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

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

where $V(q)$ 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

$$\Sigma^{is}(12) = \frac{i}{\sqrt{2}} \sum_{q_1 q_2} \int d\mathbf{q}_1 V(q_1) V(q_2) e^{i\mathbf{q}_1 \mathbf{R}_1} e^{i\mathbf{q}_2 \mathbf{R}_2} \left( \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \right) G(12)$$  \hspace{1cm} (2.72)
2.5 Closed Set of Equations

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

\[
\left\langle \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \right\rangle = \left\langle \sum_{i=j} e^{-i(\mathbf{q}_1 + \mathbf{q}_2) \mathbf{R}_i} \right\rangle + \left\langle \sum_{i \neq j} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \right\rangle
\]

(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

\[
\langle \sum_{ij} e^{-i\mathbf{q}_1 \mathbf{R}_i} e^{-i\mathbf{q}_2 \mathbf{R}_j} \rangle = N_i \delta_{\mathbf{q}_1 + \mathbf{q}_2 = 0} + N_i(N_i - 1)\delta_{\mathbf{q}_1 = 0}\delta_{\mathbf{q}_2 = 0}
\]

(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

\[
\Sigma^{is}(12) = \frac{\rho}{\pi} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} G(12) = \frac{\rho}{\pi} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} G(12).
\]

(2.75)

\( \rho \) 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

\[
\begin{align*}
\Sigma^{is}_{nm}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{n_{m1}}(\mathbf{q}_z) M'^{is}_{m_{m1}} G_{n_1 m_1}^s (\mathbf{k} - \mathbf{q}_z; t_1 t_2) . \\
\Sigma^{<is}_{nm}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{n_{m1}}(\mathbf{q}_z) M'^{<is}_{m_{m1}} G_{n_1 m_1}^< (\mathbf{k} - \mathbf{q}_z; t_1 t_2) . \\
\Sigma^{Ris}_{nm}(\mathbf{k}; t_1 t_2) &= \frac{\rho}{\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{n_{m1}}(\mathbf{q}_z) M'^{Ris}_{m_{m1}} G_{n_1 m_1}^R (\mathbf{k} - \mathbf{q}_z; t_1 t_2) . \\
\end{align*}
\]

(2.76)

The matrix elements \( M'_{n_{m1}}(\mathbf{q}_z) \) and \( M'^{is}_{m_{m1}} \) 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

\[
\begin{align*}
\Sigma^{<is}_{nm}(\mathbf{k}; E) &= \frac{\rho}{\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{n_{m1}}(\mathbf{q}_z) M'^{<is}_{m_{m1}} G_{n_1 m_1}^< (\mathbf{k} - \mathbf{q}_z; E) . \\
\Sigma^{Ris}_{nm}(\mathbf{k}; E) &= \frac{\rho}{\pi} \sum_{n_1 m_1} \sum_{\mathbf{q}} V(\mathbf{q}) V(-\mathbf{q}) M'_{n_{m1}}(\mathbf{q}_z) M'^{Ris}_{m_{m1}} G_{n_1 m_1}^R (\mathbf{k} - \mathbf{q}_z; E) . \\
\end{align*}
\]

(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

$$
\begin{pmatrix}
E - h_{CC} + i0^+ & 0 \\
0 & E - h_{LL} + i0^+
\end{pmatrix}
\begin{pmatrix}
G_R^{CC} & G_R^{CL} \\
G_R^{LC} & G_R^{LL}
\end{pmatrix}
= 
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
$$

(2.78)

where all the functions are matrices, $\Sigma_{CL}$ and $\Sigma_{LC}$ 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 $h_{nm}, n \neq m, E - h_{CC} + i0^+ = \tilde{G}^{-1}_0C$, and $E - h_{LL} + i0^+ = \tilde{G}^{-1}_0L$. $\tilde{G}_0C$ 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 $G_R^{LC}$, one obtains

$$
\tilde{G}_0L^{-1}g_R^{LC} = U_{LC}G_R^{CC} + (U_{LL} + \Sigma_{LL})G_R^{LC}
$$

(2.79)

or

$$
G_R^{LC} = \tilde{G}_0L U_{LC}G_R^{CC} + \tilde{G}_0L (U_{LL} + \Sigma_{LL})G_R^{LC}
= (\tilde{G}_0L + \tilde{G}_0L (U_{LL} + \Sigma_{LL})\tilde{G}_0L
+ \tilde{G}_0L (U_{LL} + \Sigma_{LL})^2\tilde{G}_0L (U_{LL} + \Sigma_{LL})\tilde{G}_0L + \cdots)U_{LC}G_R^{CC}
$$

(2.80)

where the second line is obtained by reiterating $G_R^{LC}$. $g_R^{LL}$ is the lead Green’s function when the lead and the device are separated (but to compute $\Sigma_{LL}$, the Green’s functions in the device should be known)

$$
g_R^{LL} = \tilde{G}_0L + \tilde{G}_0L (U_{LL} + \Sigma_{LL})g_R^{LL}.
$$

(2.81)

The equation for $G_R^{CC}$ is given by

$$
G_R^{CC} = \tilde{G}_0C + \tilde{G}_0C U_{CC} G_R^{CC} + \tilde{G}_0C U_{CL} G_R^{LC} + \tilde{G}_0C \Sigma_{CC} G_R^{CC}
= \tilde{G}_0C (1 + U_{CL} G_R^{LC}) + \tilde{G}_0C (U_{CC} + \Sigma_{CC}) G_R^{CC}
$$

$$
= g_R^{CC} (1 + U_{CL} G_R^{LC})
= g_R^{CC} + g_R^{CC} U_{CL} g_R^{LL} U_{LC} G_R^{CC}.
$$

(2.82)

The third equality results from the same procedure as for $G_R^{LC}$ where $g_R^{CC}$ is the device Green’s function when the leads are not coupled

$$
g_R^{CC} = \tilde{G}_0C + \tilde{G}_0C (U_{CC} + \Sigma_{CC}^{CC})g_R^{CC}.
$$

(2.83)
2.6 Boundary Conditions \[3\]

The iteration procedure gives the following expression for \(G_{LL}^R\)
\[
G_{LL}^R = g_{LL}^R (1 + U_{LC} G_{CL}^R).
\] (2.84)

It remains to evaluate \(G_{CL}^R\), for which one has to consider the commutative rule
\[
HG^R = G^R H
\]
\[
\begin{pmatrix}
G_{CC}^R & G_{CL}^R \\
G_{LC}^R & G_{LL}^R
\end{pmatrix}
\begin{pmatrix}
E - h_{CC} + i 0^+ \\
0
\end{pmatrix}
\begin{pmatrix}
0 \\
E - h_{LL} + i 0^+
\end{pmatrix}
= \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\]
\[+ \begin{pmatrix}
G_{CC}^R & G_{CL}^R \\
G_{LC}^R & G_{LL}^R
\end{pmatrix}
\begin{pmatrix}
U_{CC} & U_{CL} \\
U_{LC} & U_{LL}
\end{pmatrix}
+ \begin{pmatrix}
\Sigma_{CC}^R & 0 \\
0 & \Sigma_{LL}^R
\end{pmatrix}.
\] (2.85)

This gives for \(G_{CL}^R\)
\[
G_{CL}^R = G_{CC}^R U_{CL} \tilde{g}_{0L} + G_{CL}^R (U_{LL} + \Sigma_{LL}^R) \tilde{g}_{0L}
= G_{CC}^R U_{CL} (\tilde{g}_{0L} + \tilde{g}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{g}_{0L}
+ \tilde{g}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{g}_{0L} (U_{LL} + \Sigma_{LL}^R) \tilde{g}_{0L} + \cdots)
= G_{CC}^R U_{CL} g_{LL}^R
\] (2.86)

The contact properties are included in the lead Green’s function \(g_{LL}^L\), 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,
\[
G_{CC}^< = G_{CC}^R \Sigma_{CC}^< G_{CC}^A + g_{LL}^R \Sigma_{LL}^< G_{CL}^A
= G_{CC}^R \Sigma_{CC}^< G_{CC}^A + G_{CC}^R U_{CL} g_{LL}^R \Sigma_{LL}^< U_{LC} G_{CC}^A \\
= G_{CC}^R \Sigma_{CC}^< G_{CC}^A + G_{CC}^R U_{CL} g_{LL}^R U_{LC} G_{CC}^A
\]
\[
G_{CL}^< = G_{CC}^R \Sigma_{CC}^< G_{CL}^A + g_{LL}^R \Sigma_{LL}^< G_{LL}^A
= G_{CC}^R \Sigma_{CC}^< G_{CC}^A U_{CL} g_{LL}^R + G_{CC}^R U_{CL} g_{LL}^R \Sigma_{LL}^< g_{LL}^R (1 + U_{LC} G_{CL}^A) \\
= G_{CC}^R U_{CL} g_{LL}^A + G_{CC}^R U_{CL} g_{LL}^<
\]
\[
G_{LC}^< = G_{LL}^R \Sigma_{LL}^< G_{LC}^A + g_{LL}^R \Sigma_{LL}^< G_{CC}^A
= (1 + U_{LC} G_{CL}^A) g_{LL}^R \Sigma_{LL}^< g_{LL}^A U_{LC} G_{CC}^A + g_{LL}^R U_{LC} G_{CC}^R \Sigma_{CC}^< G_{CC}^A \\
= g_{LL}^R U_{LC} G_{CC}^A + g_{LL}^R U_{LC} G_{CC}^<
\]
\[
G_{LL}^< = G_{LL}^R \Sigma_{LL}^< G_{LL}^A + g_{LL}^R \Sigma_{LL}^< G_{CL}^A
= \frac{g_{LL}^R \Sigma_{LL}^< g_{LL}^A}{1} + \frac{g_{LL}^R U_{LC} G_{CC}^R U_{CL} g_{LL}^R \Sigma_{LL}^< g_{LL}^A}{1b}
\]
and stationary regime, one finds for the carrier density with equations (2.25) and (2.26).

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 (2.26): \(n(z) = \frac{i}{\hbar} \sum_{k_{\perp}, \sigma} \sum_{n,m} \frac{dE}{2\pi} G_{nm}^{<}(k_{\perp}; E) \phi_{k_{\perp}n}(z) \phi_{k_{\perp}m}^{\ast}(z),\) (2.89)

where \(\sigma\) 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 \(\rho(z, t)\)

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

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

\[
\frac{d}{dt} \rho(z, t) = \lim_{\epsilon \to 0} (-i\hbar)e \left( \frac{d}{dt} G_{nm}^{<}(z, t, t') + \frac{d}{dt'} G_{nm}^{<}(z, t, t') \right). \tag{2.91}
\]

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

\[
\frac{d}{dt} \rho_{n}(t) = \frac{e}{A \Delta} \sum_{k_{\perp}, \sigma} \frac{d}{dt} \langle a_{n,k_{\perp}}^{\dagger}(t) a_{n,k_{\perp}}(t) \rangle, e > 0 \text{ for } h, e < 0 \text{ for } \text{el.}
\]

\[
= \lim_{\epsilon \to 0} (-i\hbar) \frac{e}{A \Delta} \sum_{k_{\perp}, \sigma} \left( \frac{d}{dt} G_{nm}^{<}(k_{\perp}; t) + \frac{d}{dt'} G_{nm}^{<}(k_{\perp}; t') \right)
\]

\[
= -\frac{J_{n}(t) - J_{n-1}(t)}{\Delta}. \tag{2.92}
\]

where \(a_{n,k_{\perp}}^{\dagger}\) creates an electron at position \(z_n\), state \(k_{\perp}\), and time \(t\) (within a volume \(V = A \Delta\)), \(a_{n,k_{\perp}}(t)\) 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 \( G_{nm}^<(\mathbf{k}_t; tt') \) are required. They can be found in equations (2.34) and (2.35) and inserted into (2.92)

\[
\frac{d}{dt} \rho_n(t) = -\frac{e}{A\Delta} \sum_{k_t,\sigma} \sum_m \left\{ (h_{nm} G_{mn}^<(\mathbf{k}_t; tt) - G_{nm}^<(\mathbf{k}_t; tt) h_{mn}) + \int dt_2 \left[ (\Sigma_{nm}^R(\mathbf{k}_t; tt_2) G_{mn}^<(\mathbf{k}_t; t_2t) + \Sigma_{nm}^<(\mathbf{k}_t; tt_2) G_{mn}^A(\mathbf{k}_t; t_2t)) - \left[ G_{nm}^R(\mathbf{k}_t; tt_2) \Sigma_{nm}^<(\mathbf{k}_t; t_2t) + G_{nm}^<(\mathbf{k}_t; tt_2) \Sigma_{mn}^A(\mathbf{k}_t; t_2t) \right] \right] \right\}
\]

\[
= 0, \text{ because of condition (G.6)}
\]

(2.93)

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

\[
J_n(t) \propto \sum_{l \geq n+1} \sum_{m \leq n} T_{lm} \langle a_l^\dagger a_m \rangle - \sum_{l \leq n} \sum_{m \geq n+1} T_{lm} \langle a_l^\dagger a_m \rangle
\]

(2.94)

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

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

(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
\[ J_n = \frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{k_{l,\sigma}} \int \frac{dE}{2\pi} \left( h_{lm} G_{ml}^<(k_l; E) - G_{ml}^<(k_l; E) h_{ml} \right) \]

\[ = \frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{k_{l,\sigma}} \int \frac{dE}{2\pi} 2\text{Re} \left\{ h_{lm} G_{ml}^<(k_l; E) \right\}. \tag{2.96} \]

The second line is obtained with the help of equation (2.45). The boundary conditions from section 2.6 allow a simplification for \( G_{ml}^<(k_l; E) \), 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 \( h_{ml,lm} \). Hence, one obtains for the lesser Green’s function

\[ G_{ml}^<(k_l; E) = \sum_{l \geq n+1} \sum_{m \leq n} \left( g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E) \right) \]

\[ + g_{mm_1}^R(k_l; E) h_{m_1l} G_{l_1l}^<(k_l; E) \] \tag{2.97}

and for the current density

\[ J_n = \frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{m \leq n} \sum_{k_{l,\sigma}} \int \frac{dE}{2\pi} \left( \frac{J_{nm}^{p_1}}{J_{nm}^{p_2}} (k_l; E) \right) \]

\[ = 2\text{Re} \left\{ h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E) \right\} \]

\[ + 2\text{Re} \left\{ h_{lm} g_{mm_1}^R(k_l; E) h_{m_1l} G_{l_1l}^<(k_l; E) \right\} \]

\[ + 2\text{Re} \left\{ h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^R(k_l; E) \right\} \]

\[ + 2\text{Re} \left\{ h_{lm} g_{mm_1}^R(k_l; E) h_{m_1l} G_{l_1l}^R(k_l; E) \right\} \]

\[ \tag{2.98} \]

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. (3.13))

\[ g_{mm_1}^< (k_l; E) = if^{\text{Cont}}(E) A_{mm_1}(k_l; E), \tag{2.99} \]

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

\[ 2\text{Re} \left\{ h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E) \right\} = J_{nm}^{p_1} (k_l; E) \]

\[ = h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E) + \]

\[ (h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E)) \]

\[ = h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E) + \]

\[ (h_{lm} g_{mm_1}^<(k_l; E) h_{m_1l} G_{l_1l}^A(k_l; E)) \]
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

\[
J_{mn,l_1}^{p1}(k_t;E) = h_{lm}g_{mm_1}^<(k_t;E)h_{m_1,l_1}G_{l_1}^{g^p}(k_t;E)
- h_{m_1,l_1}g_{mm_1}^<(k_t;E)h_{lm}G_{l_1}^{g^p}(k_t;E)
- f^{Cont}(E)h_{lm}A_{mm_1}(k_t;E)h_{m_1,l_1}i\left(G_{l_1}^{r}(k_t;E) - G_{l_1}^{g^p}(k_t;E)\right)
- f^{Cont}(E)h_{lm}A_{mm_1}(k_t;E)h_{m_1,l_1}A_{l_1}(k_t;E).
\]

(2.101)

The same argumentation is also applied to the second part of equation (2.98)

\[
J_{mn,l_1}^{p2}(k_t;E)
= 2Re\left\{ h_{lm}g_{mm_1}^<(k_t;E)h_{m_1,l_1}G_{l_1}^{g^p}(k_t;E) \right\}
- h_{lm}A_{mm_1}(k_t;E)h_{m_1,l_1}iG_{l_1}^{g^p}(k_t;E)
\]

(2.102)

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

\[
J_n = \frac{e}{\hbar A} \sum_{l \geq n+1} \sum_{l_1 \geq n+1} \sum_{k_t,\sigma} \int \frac{dE}{2\pi} \Gamma^{Cont}_{ll_1}(k_t;E) \left( f^{Cont}(E)A_{ll_1}(k_t;E) + iG_{ll_1}^{g^p}(k_t;E) \right)
\]

(2.103)

with

\[
\Gamma^{Cont}_{ll_1}(k_t;E) = \sum_{m \leq n} \sum_{m_1 \leq n} h_{lm}A_{mm_1}(k_t;E)h_{m_1,l_1}.
\]

(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)

\[
J_L = \frac{e}{\hbar A} \sum_{l=1}^{N} \left( \sum_{l_1=1}^{N} \sum_{k_{l_1},\sigma} \int \frac{dE}{2\pi} \Gamma^{L}_{l_{1}l}(k_{l}; E) \left( f^{L}(E) A_{l_{1}l}(k_{l}; E) + iG^{<}_{l_{1}l}(k_{l}; E) \right) \right).
\]

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 \( J_R) \)

\[
J_R = -\frac{e}{\hbar A} \sum_{l=1}^{N} \left( \sum_{l_1=1}^{N} \sum_{k_{l_1},\sigma} \int \frac{dE}{2\pi} \Gamma^{R}_{l_{1}l}(k_{l}; E) \left( f^{R}(E) A_{l_{1}l}(k_{l}; E) + iG^{<}_{l_{1}l}(k_{l}; E) \right) \right).
\]

The index \( R \) in \( \Gamma^{R}_{l_{1}l} \) 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

\[
J = \left( \frac{J_L + J_R}{2} \right)
= \frac{e}{\hbar A} \sum_{l=1}^{N} \left( \sum_{l_1=1}^{N} \sum_{k_{l_1},\sigma} \int \frac{dE}{2\pi} \left\{ \left( \Gamma^{L}_{l_{1}l}(k_{l}; E) f^{L}(E) - \Gamma^{R}_{l_{1}l}(k_{l}; E) f^{R}(E) \right) A_{l_{1}l}(k_{l}; E) \right. \right.
+ \left. i \left( \Gamma^{R}_{l_{1}l}(E) - \Gamma^{L}_{l_{1}l}(E) \right) G^{<}_{l_{1}l}(k_{l}; E) \right\}.
\]

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 \( A_{l_{1}l}(k_{l}; E) \) and the lesser Green’s function \( G^{<}_{l_{1}l}(k_{l}; E) \) with the help of the boundary conditions described in section 2.6. After some algebra, one obtains

\[
G^{<}_{l_{1}l} = \sum_{l_2,l_3} \left( \sum_{m_{1},m_{2}} G^{R}_{l_1 l_2} h_{l_2 m_1} g^{<}_{m_1 m_2} h_{m_2 l_3} G^{A}_{l_3 l} + \sum_{m_3,m_4} G^{R}_{l_1 l_2} h_{l_2 m_3} g^{<}_{m_3 m_4} h_{m_4 l_3} G^{A}_{l_3 l} \right),
\]

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

\[ \sum_{m_1, m_2} h_{l_1m_1} g_{m_1m_2}^c h_{m_2l_3} = \sum_{m_1, m_2} i f^L h_{l_1m_1} A_{m_1m_2} h_{m_2l_3} = i f^L \Lambda_{l_2l_3} \]

\[ \sum_{m_3, m_4} h_{l_2m_3} g_{m_3m_4} h_{m_4l_3} = \sum_{m_3, m_4} i f^R h_{l_2m_3} A_{m_3m_4} h_{m_4l_3} = i f^R \Lambda_{l_2l_3} \]

and as consequence

\[ G_{l_1l}^c = \sum_{l_2, l_3} i G_{l_1l_2}^R \left( f^L \Gamma_{l_2l_3} + f^R \Gamma_{l_2l_3}^R \right) G_{l_3l}^A. \] (2.105)

Similarly, for the spectral function \( A_{l_1l} \), one obtains

\[ A_{l_1l} = i \left( G_{l_1l}^c - G_{l_1l}^\ast \right) \]

\[ = \sum_{l_2, l_3} \left( \sum_{m_1, m_2} G_{l_1l_2}^R h_{l_2m_1} A_{m_1m_2} h_{m_2l_3} G_{l_3l}^A \right) \]

\[ + \sum_{m_3, m_4} G_{l_1l_2}^R h_{l_2m_3} A_{m_3m_4} h_{m_4l_3} G_{l_3l}^A \] (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

\[ J = \frac{e}{\hbar A} \sum_{l_1} \sum_{l_2, l_3} \sum_{k_{\mathbf{t}}, \sigma} \int \frac{dE}{2\pi} \left[ \Gamma_{l_1l_2}^L G_{l_1l_2}^R \Gamma_{l_2l_3}^R G_{l_3l}^A \right] (k_{\mathbf{t}}; E) \left( f^L(E) - f^R(E) \right), \] (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 \( G_{l_1l}^c \) and \( A_{l_1l} \)

\[ G_{l_1l}^c = \sum_{l_2, l_3} G_{l_1l_2}^R \left( f^L \Gamma_{l_2l_3}^L + i f^R \Gamma_{l_2l_3}^R + \Sigma_{l_2l_3}^c \right) G_{l_3l}^A. \]

\[ A_{l_1l} = \sum_{l_2, l_3} G_{l_1l_2}^R \left( \Gamma_{l_2l_3}^L + \Gamma_{l_2l_3}^R + i \left( \Sigma_{l_2l_3}^c - \Sigma_{l_2l_3}^\ast \right) \right) G_{l_3l}^A. \] (2.108)
The interactions like carrier-phonon scattering are cast into the self-energies \( \Sigma_{l_2l_3}^< \) and \( \Sigma_{l_2l_3}^> \). The new equations (2.108) for the Green’s function \( G_{l_1l}^R \) and for the spectral function \( A_{l_1l} \) cause a two-part current density \( J \)

\[
J = J_{coh} + J_{in},
\]

(2.109)

where \( J_{coh} \) is given by equation (2.107), but its value is different from the one in the previous section because \( G_{l_1l_2}^R \) and \( G_{l_3}^I \) are calculated in the presence of interaction. The evaluation of \( J_{in} \) yields

\[
J_{in} = \frac{ie}{\hbar A} \sum_{l_1} \sum_{l_2l_3} \sum_{k_{l1},\sigma} \int \frac{dE}{2\pi} \Gamma_{l_1l_2}^L(k_{l1};E)G_{l_1l_2}^R(k_{l1};E) \left\{ \Sigma_{l_2l_3}^>(k_{l1};E)f^L(E) + \Sigma_{l_2l_3}^< (k_{l1};E)(1 - f^L(E)) \right\} G_{l_3l}^A(k_{l1};E)
\]

\[
= \frac{ie}{\hbar A} \sum_{l_1l_2l_3} \sum_{m_1m_2} \sum_{k_{l1},\sigma} \int \frac{dE}{2\pi} h_{l_1m_1}A_{m_1m_2}(k_{l1};E)h_{m_2l_1}G_{l_1l_2}^R(k_{l1};E)G_{l_3l}^A(k_{l1};E)
\]

\[
\times \left\{ \Sigma_{l_2l_3}^>(k_{l1};E)f^L(E) + \Sigma_{l_2l_3}^< (k_{l1};E)(1 - f^L(E)) \right\}
\]

\[
= \frac{e}{\hbar A} \sum_{l_1l_2l_3} \sum_{m_1m_2} \sum_{k_{l1},\sigma} \int \frac{dE}{2\pi} h_{l_1m_1}h_{m_2l_1}G_{l_1l_2}^R(k_{l1};E)G_{l_3l}^A(k_{l1};E)
\]

\[
\times \left\{ \Sigma_{l_2l_3}^>(k_{l1};E)g_{m_1m_2}^<(k_{l1};E) - \Sigma_{l_2l_3}^< (k_{l1};E)g_{m_1m_2}^>(k_{l1};E) \right\},
\]

(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 \( \tau \) which can be energy-dependent or not. This gives for the retarded self-energy \( \Sigma_{nm}^R(k_{l1};E) \) (unit [eV]) assuming that it is only diagonal

\[
\Sigma_{nm}^R(k_{l1};E) = -i\frac{\hbar}{\tau}\delta_{nm}.
\]

(2.111)

Because of the current condition presented in Appendix G, the lesser self-energy \( \Sigma_{nm}^<(k_{l1};E) \) cannot be chosen without restriction, but must be diagonal and must
fulfill
\[
\sum_{k_t} \int dE \left( \Sigma_{nn}^R(k_t; E) G_{nn}^\le (k_t; E) + \Sigma_{nn}^\le (k_t; E) G_{nn}^A (k_t; E) \right)
\]
\[= G_{nn}^R (k_t; E) \Sigma_{nn}^\le (k_t; E) - \Sigma_{nn}^\le (k_t; E) \Sigma_{nn}^A (k_t; E) \]  (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

\[G_{nn}^\le (k_t; E) = i f(E) A_{nn} (k_t; E), \quad \Sigma_{nn}^\le (k_t; E) = i (G_{nn}^R (k_t; E) - G_{nn}^A (k_t; E)),\]
\[A_{nn} (k_t; E) = i (G_{nn}^R (k_t; E) - G_{nn}^A (k_t; E)), \quad \Sigma_{nn}^\le (k_t; E) = i (G_{nn}^R (k_t; E) - G_{nn}^A (k_t; E)).\]

\(f(E)\) 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
\[\Sigma_{nn}^\le (k_t; E) = i f_n(E) \Gamma_{nn} (k_t; E)\]
\[= 2i f_n(E) \hbar. \]  \hspace{1cm} (2.133)

Taking this into account, with some simple algebra and previously defined relations for the Green’s functions, condition (2.112) becomes
\[\sum_{k_t} \int dE \left( G_{nn}^\le (k_t; E) (\Sigma_{nn}^R (k_t; E) - \Sigma_{nn}^A (k_t; E)) \right)
\]
\[= \sum_{k_t} \int dE \left( G_{nn}^\le (k_t; E) \Sigma_{nn}^\ge (k_t; E) - \Sigma_{nn}^\le (k_t; E) G_{nn}^\ge (k_t; E) \right) =
\]
\[= \sum_{k_t, m} \int dE \left( G_{nm}^R (k_t; E) \frac{\Sigma_{mn}^\le (k_t; E)}{i f_m(E) \Gamma_{mn} (k_t; E)} \frac{G_{mn}^A (k_t; E)}{i (f_m(E) - 1) \Gamma_{mn} (k_t; E)} \right)
\]
\[= \sum_{k_t, m} \int dE T^{nm}(k_t; E) \left( f_m(E) - f_n(E) \right) = 0 \quad (2.114)\]

with
\[T^{nm}(k_t; E) = \frac{\Gamma_{nm} (k_t; E) G_{nn}^R (k_t; E) \Gamma_{mn} (k_t; E) G_{mn}^A (k_t; E)}{\Gamma_{nn} (k_t; E) G_{nn}^R (k_t; E) \Gamma_{mm} (k_t; E)}. \]  \hspace{1cm} (2.115)

\(T^{nm}(k_t; E)\) 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

\[
J_n = -\frac{e}{h A} \sum_{k, \sigma} \int \frac{dE}{2\pi} \left( h_{n+1n} G_{n+1n}^>(k_t; E) - G_{n+1n}^<(k_t; E) h_{n+1n} \right).
\]  

(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 \( g(k_t; E) \) come form the leads (all the points except \( n+1 \)) and the big ones \( G(k_t; E) \) from the device. The variables \( k_t \) and \( E \) are neglected if they do not contribute to the signification of the equation. This leads to

\[
G_{n+1n}^<(\equiv G_{LC}^<) = g_{n+1n}^< h_{n+1n}^A G_{n+1n+1}^A + g_{n+1n}^R h_{n+1n}^A G_{n+1n+1}^<
\]

\[
G_{n+1n}^< (\equiv G_{CL}^<) = G_{n+1n+1}^A h_{n+1n}^A + G_{n+1n+1}^R h_{n+1n}^A
\]  

(2.117)

and therefore

\[
h_{n+1n} G_{n+1n+1}^< - G_{n+1n}^< h_{n+1n+1} = h_{n+1n} g_{n+1n}^< h_{n+1n+1} \left( G_{n+1n+1}^A - G_{n+1n+1}^R \right) +
\]

\[
h_{n+1n} \left( g_{n+1n}^R - g_{n+1n}^A \right) h_{n+1n+1} G_{n+1n+1}^<
\]

\[
= h_{n+1n} g_{n+1n}^< h_{n+1n+1} G_{n+1n+1}^< - h_{n+1n} g_{n+1n}^< h_{n+1n+1} G_{n+1n+1}^R.
\]  

(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

\[
g_{n+1n}^< = \sum_{m_1 < n+1} g_{nm_1}^R \sum_{m_1 m_1 n} g_{m_1 n}^A.
\]
so that one has \( \text{tions (2.122) and (2.123), the expression (2.120) can be further simplified and one}

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))

\[
J_{n+\frac{1}{2}} = -\frac{e}{\hbar} \sum_{\mathbf{k}_t \sigma} \sum_{m_1 < n+1} \sum_{m_2 \geq n+1} \int dE \left[ \Gamma_{m_1 m_1}^R \Gamma_{m_1 m_2} \Gamma_{m_2 m_2}^{A} \right] (\mathbf{k}_t; E) \left( f_{m_2}(E) - f_{m_1}(E) \right). 
\]

(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 $\Sigma$ while the effects of the contacts are taken into account exactly through a boundary self-energy $\Sigma^B$.

All these effects are included in the Hamiltonian given by

$$H = H_0 + H_{opp} + H_{acp} + H_{ir} + H_{al} + H_{id},$$  \hspace{1cm} (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 $H^{DR}$)

$$H_0 = H^D + H^L_0 + H^R_0 + H^{DL}_0 + H^{DR}_0.$$ (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

$$H_0 = -\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + \frac{\hbar^2 k_i^2}{2m^*} + V(z)$$ (3.3)
and as consequence, $h_{nm}$ from equation (2.45) becomes

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

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

$$\sum_l h_{nl} G_{lm}^R (k_t; t_1 t_2) =$$

$$\int dz_1 \int dz_2 \phi_n^*(z_1) \left( -\frac{\hbar^2}{2m^*} \nabla^2 + V(z_1) + \frac{\hbar^2 k_t^2}{2m^*} \right) G(k_t; z_1; z_2) \phi_m(z_2) =$$

$$\int dz_1 \phi_n^*(z_1) \left[ \left( \frac{\hbar^2}{m^* \Delta^2} + V(z_1) + \frac{\hbar^2 k_t^2}{2m^*} \right) G_m(k_t; z_1; t_2) - \right.$$

$$\left. \frac{\hbar^2}{2m^* \Delta^2} (G_m(k_t; z_1 + \Delta; t_1 t_2) + G_m(k_t; z_1 - \Delta; t_1 t_2)) \right] =$$

$$\sum_{n_1} \int dz_1 \phi_n^*(z_1) \left[ \left( \frac{\hbar^2}{m^* \Delta^2} + V(z_1) + \frac{\hbar^2 k_t^2}{2m^*} \right) G_{n_1m}(k_t; t_1 t_2) - \right.$$

$$\left. \frac{\hbar^2}{2m^* \Delta^2} (G_{n_1+1m}(k_t; t_1 t_2) + G_{n_1-1m}(k_t; t_1 t_2)) \right) \phi_{n_1}(z_1) =$$

$$D_n G_{nm}(k_t; t_1 t_2) - t_{n+1} G_{n+1m}(k_t; t_1 t_2) - t_{n-1} G_{n-1m}(k_t; t_1 t_2).$$

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

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

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

$$G_{ij}^R = g_{ij}^R + g_{i1}^R \left( -t_{10} \right) g_{10}^R (-t_{01}) G_{ij}^R + g_{iN}^R \left( -t_{NN+1} \right) g_{N+1N}^R (-t_{N+1N}) G_{Nj}^R.$$ 

$$\sum_{i=1}^{N} \sum_{j=1}^{N} (3.6)$$
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. $t_{10}$, $t_{01}$, $t_{N+1}$, and $t_{N+1}$ are set to zero. For instance, $g_{ij}^R$ obeys the following equation, combination of (2.45) and (2.83)

\[
\sum_{l \in N} \left[ (E - D_l) \delta_{il} + t_{il} - \Sigma^R_{il} \right] g_{ij}^R = \delta_{ij}, \tag{3.7}
\]

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

\[
\sum_{l \in N} \left[ (E - D_l) \delta_{il} + t_{il} - \Sigma^R_{il} \right] G_{ij}^R = \delta_{ij} + \delta_{i1} \Sigma^R_{11} G_{1j}^R + \delta_{iN} \Sigma^R_{NN} G_{Nj}^R \tag{3.8}
\]

This equation can be rewritten in matrix form as follows

\[
[g^R] = \left( \begin{array}{cccccc}
E - D_1 - \Sigma^R_{11} & t_{12} - \Sigma^R_{21} & -\Sigma^R_{13} & \cdots & -\Sigma^R_{1N-1} & -\Sigma^R_{1N} \\
t_{21} - \Sigma^R_{21} & E - D_2 - \Sigma^R_{22} & t_{23} - \Sigma^R_{32} & \cdots & -\Sigma^R_{2N-1} & -\Sigma^R_{2N} \\
-\Sigma^R_{31} & t_{32} - \Sigma^R_{32} & E - D_3 - \Sigma^R_{33} & \cdots & -\Sigma^R_{3N-1} & -\Sigma^R_{3N} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
-\Sigma^R_{N1} & -\Sigma^R_{N2} & -\Sigma^R_{N3} & \cdots & E - D_{N-1} - \Sigma^R_{N-1} & t_{N-1} - \Sigma^R_{NN} \\
-\Sigma^R_{N1} & -\Sigma^R_{N2} & -\Sigma^R_{N3} & \cdots & t_{N+1} - \Sigma^R_{NN-1} & E - D_N - \Sigma^R_{NN} - \Sigma^R_{NN} \\
\end{array} \right)^{-1}.
\]

In the first part of Lake’s paper [4], all the interaction self-energies $\Sigma^R$ were set equal to 0 and only the boundary self-energies $\Sigma^R_{11}$ and $\Sigma^R_{NN}$ 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 $\Sigma^R_{11}$ and $\Sigma^R_{NN}$. In order to get them, one recalls equation (2.81) from section 2.6 and sets $\Sigma^R_{LL}$ equal to 0. One has therefore for the left reservoir

\[
\sum_{\gamma = -N_L+1}^{0} \left[ (E - D_\alpha) \delta_{\alpha\gamma} + t_{\alpha\gamma} \right] g^R_{\gamma\beta} = \delta_{\alpha\beta}. \tag{3.9}
\]

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

\[
(E - D_{-N_L+1})g_{-N_L+1,-N_L+1}^R + t_{-N_L+1,-N_L+1}g_{-N_L+1,-N_L+2}g_{-N_L+2,-N_L+1} \]

\[
\cdots + t_{-N_L+1,-N_L}g_{-N_L,-N_L+1} + \Sigma^R_{-N_L+1,-N_L+1} = 1, \tag{3.10}
\]

where $\Sigma^R_{-N_L+1,-N_L+1} = (-t_{-N_L+1,-N_L})g_{-N_L,-N_L}^R(-t_{-N_L,-N_L+1})$ represents the coupling with the lead after Eq. (2.82) and $g_{-N_L,-N_L}$ is the first Green’s function in
the lead when lead and reservoir are not coupled \((\gamma_{-N_L,-N_L+1} = \gamma_{-N_L+1,-N_L} = 0)\). It will be evaluated with the following assumptions: the potential for layers \(\gamma = [-\infty, \cdots, -N_L]\) 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. \(g_{N\beta} \propto e^{ik_e|\alpha-\beta|\Delta}\) (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

\[
\begin{align*}
g^{R}_{-N_L,2,-N_L} &= e^{ik_e\Delta}g^{R}_{-N_L,1,-N_L} \\
g^{R}_{-N_L,1,-N_L} &= e^{ik_e\Delta}g^{R}_{-N_L,-N_L}.
\end{align*}
\tag{3.11}
\]

Inserting these results into Dyson’s equation for \(g^{R}_{-N_L,-N_L}\) and \(g^{R}_{-N_L-1,-N_L}\) yields

\[
\begin{align*}
(E - D_{-N_L})g^{R}_{-N_L,-N_L} + t_{-N_L,-N_L-1} g^{R}_{-N_L-1,-N_L} e^{ik_e\Delta}g^{R}_{-N_L,-N_L} \\
+ t_{-N_L,-N_L-1} g^{R}_{-N_L+1,-N_L} &= 1
\end{align*}
\]

\[
\begin{align*}
(E - D_{-N_L-1})g^{R}_{-N_L-1,-N_L} + t_{-N_L-1,-N_L} g^{R}_{-N_L,-N_L} e^{ik_e\Delta}g^{R}_{-N_L-1,-N_L} \\
+ t_{-N_L-1,-N_L-2} g^{R}_{-N_L-2,-N_L} e^{ik_e\Delta}g^{R}_{-N_L-1,-N_L} &= 0. \tag{3.12}
\end{align*}
\]

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

\[
\begin{align*}
(E - D_{-N_L} + t_e e^{ik_e\Delta})g^{R}_{-N_L,-N_L} &= 1 \\
(E - D_{-N_L} + t_e e^{ik_e\Delta} + t_e e^{-ik_e\Delta}) &= 0 \tag{3.13}
\end{align*}
\]

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

\[
\begin{align*}
g^{R}_{-N_L,-N_L} &= -\frac{e^{ik_e\Delta}}{t_e} \quad \text{and} \quad \Sigma^{RB}_{-N_L+1,-N_L+1} &= -t_e e^{ik_e\Delta}. \tag{3.14}
\end{align*}
\]

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

\[
k_e = \frac{1}{\Delta} \arccos\left(\frac{D_{-N_L} - E}{2t_e}\right). \tag{3.15}
\]
The calculated retarded self-energy $\Sigma^{RB}_{-N+1,-N+1}$, 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)

$$
\begin{align*}
[ g^{Re} ] &= \begin{pmatrix}
E - D_{-N+1} - \Sigma^{RB}_{-N+1,-N+1} & t_{-N+1,-N+1} & 0 & \cdots & 0 \\
0 & E - D_{-N+2} - \Sigma^{RB}_{-N+2,-N+2} & t_{-N+2,-N+2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & E - D_{-N+3} - \Sigma^{RB}_{-N+3,-N+3} \\
t_0, & 0 & 0 & \cdots & t_{0,-1} \\
\end{pmatrix}^{-1}
\end{align*}
$$

True bound states may be present in the spectrum of $g^{Re}_{00}$ (and also $g^{Re}_{NN+1N+1}$) 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

$$
G_{ij}^< = \sum_{mn} \{ G_{im}^R \Sigma_{mn}^< G_{nj}^A \} + G_{1i}^R (t_{10}) g_{00}^< (t_{01}) G_{1j}^A \\
+ G_{iN}^R (t_{N+1N+1}) g_{NN+1N+1}^< (t_{N+1N}^< N) G_{Nj}^A. \tag{3.16}
$$

$g_{00}^<$ and $g_{NN+1N+1}^<$ can be obtained from the fluctuation-dissipation theorem (section 1.3.3)

$$
\begin{align*}
g_{00}^< &= -f^e \left( g^{Re}_{00} - g^{Ac}_{00} \right) = i f^e A_{00} \\
g_{NN+1N+1}^< &= -f^e \left( g^{Re}_{NN+1N+1} - g^{Ac}_{NN+1N+1} \right) = i f^e A_{NN+1N+1} \tag{3.17}
\end{align*}
$$

and

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

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 $\Sigma^R$ and $\Sigma^<$. Some examples are available in section 2.5.3 but general expressions can also be found in
3.1 Resonant Tunneling Based Quantum Devices

3.1.1 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.

\[
n(z_n) = \frac{1}{\Delta} \int_{z_n - \frac{\Delta}{2}}^{z_n + \frac{\Delta}{2}} dz \ n(z) = -\frac{i}{\Delta A} \sum_{k_t, \sigma} \int \frac{dE}{2\pi} G^<_{nn}(k_t; E)
\]

\[
= -\frac{i}{\Delta A} \sum_{k_t, \sigma} \int \frac{dE}{2\pi} \left\{ [G^R_{n1} \Sigma^B_{11} G^A_{1n}] (k_t; E) + [G^R_{nN} \Sigma^B_{NN} G^A_{Nn}] (k_t; E) \right\}
\]

\[
= \frac{1}{\Delta A} \sum_{k_t, \sigma} \int \frac{dE}{2\pi} \left\{ f^c [G^R_{n1} \Gamma^c_{11} G^A_{1n}] (k_t; E) + f^c [G^R_{nN} \Gamma^c_{NN} G^A_{Nn}] (k_t; E) \right\}
\]

\[
= \frac{1}{\Delta A} \sum_{k_t, \sigma} \int \frac{dE}{2\pi} \left\{ (f^c - f^a) [G^R_{n1} \Gamma^c_{11} G^A_{1n}] (k_t; E) + f^c A_{nn}(k_t; E) \right\}
\]

\[
J = \frac{e}{\hbar A} \sum_{k_t, \sigma} \int \frac{dE}{2\pi} \left\{ \Gamma^c_{11} G^R_{1n} \Gamma^c_{NN} G^A_{Nn} \right\} (k_t; E) (f^c(E) - f^a(E))
\]
\[ T = \text{with } G \]

For ballistic transport, the first column and the diagonal of the matrix representing \( G \) 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 \( g \)'s 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 \( g_{0,n} \), \( t_{n-1} \) and \( t_{n-1} \) are equal to 0. The equation for \( g_{0,n;N,N} \) and \( g_{n+1,n;N,N} \) can be written as

\[
T_{n,N,n;N} g_{n,n;N,N} = 1 \quad T_{n+1,N,n;N} g_{n+1,n;N,N} = 1, \quad (3.21)
\]

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 \( \Sigma^{RR} \)'s. In matrix form, one has

\[
\begin{pmatrix}
T_{nn} & T_{n,n+1;N} \\
T_{n+1,N,n} & T_{n+1,N,n+1;N}
\end{pmatrix}
\begin{pmatrix}
g_{nn} \\
g_{n+1,n;N}
\end{pmatrix}
= \begin{pmatrix}
1 & 0_{n,n+1;N} \\
0_{n+1;N,n} & 1_{n+1;N,n,n+1;N}
\end{pmatrix}
\]

with \( T_{n,n+1;N} = [T_{nn+1} \; 0 \; \cdots \; 0] \) and \( T_{n+1;N,n} = [T_{n+1;N,n} \; 0 \; \cdots \; 0] \). One can extract two equations

\[
T_{nn} g_{nn} + T_{n,n+1;N} g_{n+1,n;N} = 1 \\
T_{n+1;N,n} g_{nn} + T_{n+1;N,n+1;N} g_{n+1,n;N} = 0_{n+1;N,n}.
\]

From the first one and the properties of \( T \) described above,

\[
T_{nn} g_{nn} + T_{n+1;N,n} g_{n+1;N,n} = 1, \quad (3.23)
\]

and from the second equation

\[
\begin{align*}
(g_{n+1;N,n+1;N})^{-1} g_{n+1;N,n} &= -T_{n+1;N,n} g_{nn} \\
g_{n+1;N,n} &= -g_{n+1;N,n+1;N} T_{n+1;N,n} g_{nn} \\
g_{n+1;N,n} &= -g_{n+1;N,n+1} T_{n+1;N,n} g_{nn}
\end{align*}
\]

The combination of both results yields

\[
g_{nn} = (T_{nn} - T_{n+1;N,n} g_{n+1;N,n+1} T_{n+1;N,n})^{-1}. \quad (3.25)
\]
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 $g$’s can be found. For the exact Green’s functions, the equation to be solved is

$$
\left( \begin{array}{cc}
T_{1:n,1:n} & T_{1:n,n+1:N} \\
T_{n+1:N,1:n} & T_{n+1:N,n+1:N}
\end{array} \right) \cdot \left( \begin{array}{cc}
G_{1:n,1:n} & G_{1:n,n+1:N} \\
G_{n+1:N,1:n} & G_{n+1:N,n+1:N}
\end{array} \right) = \left( \begin{array}{cc}
1_{1:n,1:n} & 0_{1:n,n+1:N} \\
0_{n+1:N,1:n} & 1_{n+1:N,n+1:N}
\end{array} \right)
$$

or

$$
\left( \begin{array}{cc}
G_{1:n,1:n} & G_{1:n,n+1:N} \\
G_{n+1:N,1:n} & G_{n+1:N,n+1:N}
\end{array} \right) \cdot \left( \begin{array}{cc}
T_{1:n,1:n} & T_{1:n,n+1:N} \\
T_{n+1:N,1:n} & T_{n+1:N,n+1:N}
\end{array} \right) = \left( \begin{array}{cc}
1_{1:n,1:n} & 0_{1:n,n+1:N} \\
0_{n+1:N,1:n} & 1_{n+1:N,n+1:N}
\end{array} \right).
$$

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

$$
T_{n+1:N,1:n}G_{1:n,n+1:N} + T_{n+1:N,n+1:N}G_{n+1:N,n+1:N} = 1_{n+1:N,n+1:N}
$$

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

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

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

from the second

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

and the combination of both delivers

$$
G_{n+1:N,n+1:N} = g_{n+1:N,n+1:N}
$$

$$
-g_{n+1:N,n+1:N}T_{n+1:N,1:n}G_{1:n,1:n}T_{1:n,n+1:N}g_{n+1:N,n+1:N}. \quad (3.29)
$$

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

$$
G_{n+1:n+1} = g_{n+1:n+1} + g_{n+1:n+1,N}T_{n+1:n,n+1}G_{nm}T_{mn+1}g_{n+1:n+1}. \quad (3.30)
$$

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

$$
(E - D_1)G_{1,1} + t_{12}G_{2,1} - \Sigma_{11}^R G_{1,1} = 1. \quad (3.31)
$$

From the first matrix equation above, one has

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

which can be written as

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

The isolation of the first element yields

$$
G_{n+1} = -g_{n+1:n+1}T_{n+1:n}G_{n,n+1}. \quad (3.34)
$$
Furthermore, one also needs the lesser Green’s functions for the case $n = 1$, one finds $G_{21} = -g_{22}^T T_{21} G_{11}$, one puts this result into equation (3.31), and one obtains

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

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 $T_{nn} = 0$. The equations for $g_{n:N,n:N}^{<}$ and $g_{n+1:N,n+1:N}^{<}$ are therefore

$$T_{n:N,n:N} g_{n:N,n:N}^{<} = \Sigma_{n:N,n:N}^{<} g_{n:N,n:N}^{<},$$

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

$\Sigma_{n:N,n:N}$ 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

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

Two coupled equations can be extracted from (3.37)

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

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

$$g_{n+1:N,n}^{<} = -g_{n+1:N,n+1:N}^{<} T_{n+1:N,n} g_{n:n}^{<} + g_{n+1:N,n+1:N}^{<} \Sigma_{n+1:N,n+1:N}^{<} g_{n+1:N,n+1:N}^{<}. \quad (3.39)$$
Furthermore, the lower case advanced Green’s function \( g_{n+1}^{<n} \) is given by equation (3.24)

\[
g_{n+1}^{<n} = -g_{n+1}^{A_{n+1}} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{A_{n}}.
\] (3.40)

The first part of equation (3.39) becomes

\[
\begin{align*}
(1) & : \quad g_{n+1}^{R_{n+1}} T_{n+1}^{*} g_{m}^{<n} \\
& : \quad g_{n+1}^{R_{n+1}} T_{n+1}^{*} g_{m}^{<n}
\end{align*}
\] (3.41)

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

\[
\begin{align*}
(2) & : \quad g_{n+1}^{R_{n+1}} \Sigma_{n+1}^{n+1} g_{m}^{A_{n+1}} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{A_{n}} \\
& \quad - g_{n+1}^{A_{n+1}} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{A_{n}} \\
& \quad - T_{n+1}^{*} g_{m}^{<n+1} \\
& \quad - I_{n+1}^{<n+1} \\
& : \quad g_{n+1}^{<n+1} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{A_{n}}
\end{align*}
\] (3.42)

This gives for \( g_{n+1}^{<n} \) and for its reduced form \( g_{n+1}^{<n} \)

\[
\begin{align*}
g_{n+1}^{<n} &= -g_{n+1}^{R_{n+1}} T_{n+1}^{*} g_{m}^{<n} - g_{n+1}^{<n+1} T_{n+1}^{*} g_{m}^{A_{n}} \\
g_{n+1}^{<n} &= -g_{n+1}^{R_{n+1}} T_{n+1}^{*} g_{m}^{<n} - g_{n+1}^{<n+1} T_{n+1}^{*} g_{m}^{A_{n}}.
\end{align*}
\] (3.43)

\( g_{n+1}^{<n} \) for \( g_{n+1}^{<n} \) is then inserted into the first equation of (3.60) to obtain a recursive for \( g_{m}^{<n} \) depending on \( g_{n+1}^{<n} \)

\[
\begin{align*}
\left( T_{n+1}^{*} - g_{n+1}^{R_{n+1}} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{<n} \right) g_{m}^{<n} &= T_{n+1}^{*} g_{n+1}^{<n+1} T_{n+1}^{*} g_{m}^{A_{n}} + \sum_{m_{n}} g_{m}^{A_{n}}
\end{align*}
\] (3.44)

which yields

\[
\begin{align*}
g_{n+1}^{<n} &= g_{n+1}^{R_{n+1}} T_{n+1}^{*} T_{n+1}^{*} g_{m}^{<n} + g_{n+1}^{<n+1} T_{n+1}^{*} g_{m}^{A_{n}}
\end{align*}
\] (3.45)

Starting from \( g_{N+1}^{<N} \) and going back to \( g_{N_{L}, N_{R}}^{<N} \), all the lower case Green’s functions can be obtained. For the exact Green’s functions, the equation to be solved is

\[
\begin{align*}
\begin{pmatrix}
T_{n+1}^{<n} & T_{n+1}^{<n+1} \\
T_{n+1}^{<n+1} & T_{n+1}^{<n+1}
\end{pmatrix}
& \begin{pmatrix}
C_{n+1}^{<n} \\
G_{n+1}^{<n+1}
\end{pmatrix}
= \\
\begin{pmatrix}
\Sigma_{n+1}^{<n} \\
0_{n+1}^{<n+1}
\end{pmatrix}
& \begin{pmatrix}
G_{n+1}^{<n+1} \\
G_{n+1}^{<n+1}
\end{pmatrix}
= \\
\begin{pmatrix}
G_{n+1}^{<n+1} \\
G_{n+1}^{<n+1}
\end{pmatrix}
& \begin{pmatrix}
C_{n+1}^{<n+1} \\
G_{n+1}^{<n+1}
\end{pmatrix}
\end{align*}
\] (3.46)
or
\[
\begin{pmatrix}
G_{n+1:n,1:n}^< & G_{n+1:n,1:n}^< \\
G_{n+1:n,1:n}^R & G_{n+1:n,1:n}^R
\end{pmatrix}
\begin{pmatrix}
T_{n+1:n,1:n}^s & T_{n+1:n,1:n}^s \\
T_{n+1:n,1:n}^s & T_{n+1:n,1:n}^s
\end{pmatrix}
=
\begin{pmatrix}
\sum_{1:n}^< & 0_{1:n,1:n} \\
\sum_{1:n}^> & 0_{1:n,1:n}
\end{pmatrix}
\cdot
(3.47)
\]

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 \(G_{n+1:n,n+1:N}^<\) 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
\[
\begin{align*}
T_{n+1:n,1:n}G_{n+1:n,n+1:N}^< + T_{n+1:n,1:n}N G_{n+1:n,n+1:N}^< &= \sum_{n+1:n,n+1:N}^< G_{n+1:n+1,N}^A \\
G_{1:n,1:n}^< T_{n+1:n,1:n}^* + G_{1:n,1:n}^< T_{n+1:n,1:n} = G_{1:n,n+1:N}^R \sum_{n+1:n,n+1:N}^< G_{n+1:n,1:n}^R.
\end{align*}
(3.48)
\]

One starts with the first equation of (3.48) and separates the result into two parts
\[
G_{n+1:n,n+1:N}^< = -g_{n+1:n,n+1:N}^{Rn+1} T_{n+1:n,1:n} G_{1:n,n+1:N}^< +
\]
\[
\begin{align*}
&g_{n+1:n,n+1:N}^{Rn+1} \sum_{n+1:n,n+1:N}^< G_{n+1:n,n+1:N}^R \\
&1 + T_{n+1:n,1:n}^* G_{1:n,1:n}^A T_{n+1:n,1:n}^* \sum_{n+1:n,n+1:N}^< g_{n+1:n,1:n}^{An+1} N_{n+1:n,n+1:N}.
\end{align*}
(3.49)
\]

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)
\[
(2) : \quad g_{n+1:n,n+1:N}^{Rn+1} \sum_{n+1:n,n+1:N}^< G_{n+1:n,n+1:N}^R \\
1 + T_{n+1:n,1:n}^* G_{1:n,1:n}^A T_{n+1:n,1:n}^* \sum_{n+1:n,n+1:N}^< g_{n+1:n,1:n}^{An+1} N_{n+1:n,n+1:N}.
\]

The second equation from the system developed in (3.48) is also composed of two parts
\[
G_{1:n,n+1:N}^< = -G_{1:n,1:n}^< T_{n+1:n,n+1:N}^* g_{n+1:n,1:n}^{An+1} +
\]
\[
G_{1:n,n+1:N}^R \sum_{n+1:n,n+1:N}^< g_{n+1:n,1:n}^{An+1} N_{n+1:n,n+1:N}.
(3.50)
\]

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
\[
(4) : \quad -G_{1:n,1:n}^R T_{n+1:n,n+1:N}^* g_{n+1:n,1:n}^{An+1}.
(3.51)
\]
3.1 Resonant Tunneling Based Quantum Devices

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

\[ G_{1:n,n+1:N}^< = -G_{1:n,n}^< T_{n,n+1}^* g_{n+1,n+1}^A - G_{1:n,n}^R T_{n,n+1} g_{n+1,n+1}^< \]  

(3.52)

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

\[ G_{n+1:N,n+1:N}^< = g_{n+1:N,n+1:N}^< + g_{n+1:N,n+1:N}^> T_{n,n+1}^* g_{n,n}^A T_{n,n+1}^* + g_{n+1:N,n+1:N}^< g_{n,n}^R T_{n,n+1} g_{n+1,n+1:N}^< \]  

(3.53)

or

\[ G_{n+1,n+1}^< = g_{n+1,n+1}^< + g_{n+1,n+1}^> T_{n,n+1}^* g_{n,n}^A T_{n,n+1}^* + g_{n+1,n+1}^< g_{n,n}^R T_{n,n+1} g_{n+1,n+1}^< \]  

(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.
At the end, an algorithm taking into account multiple sequential scattering is shown, enabling gain of time in the calculation but violating some physical rules, like the zero current at equilibrium but keeping the current conservation.

### 3.2 Two-dimensional Nanotransistors

The simulation of ballistic quantum transport for two-dimensional nanotransistors (metal oxide field effect transistor) is analyzed in the paper of A. Svizhenko et al. [14]. Since MOSFETs with channel lengths in the tens of nanometer regime have recently been demonstrated by various research labs, it is important to be able to simulate such devices. Despite the best modeling approach for design and analysis of nanoscale MOSFETs is presently unclear, it is generally accepted that semi-classical methods are inadequate and that quantum mechanical modeling is necessary. Svizhenko et al. present a framework for 2D quantum mechanical simulation of MOSFETs as shown in figure 3.2. They developed a nonequilibrium Green’s functions scheme solved self-consistently with Poisson’s equation.

![Figure 3.2: Nanoscale MOSFET with 2D Grid. Each column q corresponds to a submatrix of equation (3.40).](image_url)
3.2 Two-dimensional Nanotransistors

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 \( x (i'i') \) and two for \( y (jj') \), and it will depend on \( k_z \) \( G_{i'i'jj'}(k_z; t_1 t_1') \),

\[
G(11') = \frac{1}{L_z} \sum_{i'i'} \sum_{jj'} \sum_{k_z} \phi_{i'j}(xy) G_{i'i'jj'}(k_z; t't') \phi_{i'j'}^*(x'y') e^{ik_z(z-z')},
\]

\[
G_{i'i'jj'}(k_z; t't') = \int \mathrm{d}r \int \mathrm{d}r' \phi_{i'j}(xy) G(11') \phi_{i'j'}(x'y') e^{-ik_z(z-z')}, \tag{3.55}
\]

where \( \phi_{i'j}(xy) \) 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)

\[
EG_{i'i'jj'}^<(k_z; E) - \sum_{i_j1} h_{i's,jj1} G_{i'i'jj1'}^<(k_z; E) = \sum_{i_j1} \Sigma_{i'i'jj1'}^R(k_z; E) G_{i'i'jj1'}^<(k_z; E) + \sum_{i_j1} \Sigma_{i'i'jj1'}^<(k_z; E) G_{i'i'jj1'}^A(k_z; E)
\]

\[
EG_{i'i'jj'}^R(k_z; E) - \sum_{i_j1} h_{i's,jj1} G_{i'i'jj1'}^R(k_z; E) = \delta_{ii'} \delta_{jj'} + \sum_{i_j1} \Sigma_{i'i'jj1'}^R(k_z; E) G_{i'i'jj1'}^R(k_z; E)
\]

(3.56)

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

\[
H_0 = -\frac{h^2}{2 m^* x^2} \frac{d^2}{dx^2} - \frac{h^2}{2 m^* y^2} \frac{d^2}{dy^2} + \frac{h^2 k_z^2}{2 m^* z} + V(xy) \tag{3.57}
\]

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

\[
t_{i'i'}^{jj'} = \begin{cases} 
\frac{h^2}{m_j \pm 1} & \text{if } i' = i \pm 1, j' = j, \\
\frac{h^2}{m_j \mp 1} & \text{if } i' = i, j' = j \pm 1, \\
0 & \text{otherwise}
\end{cases}
\]

(3.58)
For the structure defined in figure 3.2, there are \( N \) points from 1 to \( N_x \) 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

\[
G_{ii'jj'}^R = g_{ii'jj'}^R + \sum_{i_1i_2} g_{i_1j_1}^R \left[ \begin{array}{c} 0 \\ \Sigma_{R_{i_1}S_{i_2}} \end{array} \right] \left[ \begin{array}{c} 0 \\ \Sigma_{R_{i_1}S_{i_2}} \end{array} \right] \left[ \begin{array}{c} \sum_{i_1i_2} g_{i_1j_1}^R \left( -t_{i_1j_1}^{i'j'} \right) g_{i_1j_0}^R \left( -t_{i_1j_0}^{i'j_0} \right) G_{i_2j'1j'}^R \\ \sum_{i_1i_2} g_{i_2j_2}^R \left( -t_{i_2j_2}^{i'j_2} \right) g_{i_2j_0}^R \left( -t_{i_2j_0}^{i'j_0} \right) G_{i_2j'1j'}^R \end{array} \right].
\] \tag{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, \( \Sigma_{RS} \) is the boundary self-energy for the source contact, \( \Sigma_{RD} \) for the Drain, and \( \Sigma_{RG} \) for the Gate. Furthermore, \( g_{ii'jj'}^R \) obeys the following equation, similar to (3.7), but for ballistic transport

\[
\sum_{i_0 \in N_x, j_0 \in N_y} \left[ (E - h_{i_0j_0}) \delta_{i_0i} \delta_{j_0j} + t_{i_0j_0}^{i'j'} \right] g_{i_0i'j_0j'}^R = \delta_{ii'} \delta_{jj'}. \tag{3.61}
\]

Operating with \( g^{-1}_{i_0i'j_0j'} \) on \( G_{i_0i'j_0j'}^R \) from equation (3.60) and summing over \( i_0 \) and \( j_0 \) yields

\[
\sum_{i_0 \in N_x} \sum_{j_0 \in N_y} \left[ (E - h_{i_0j_0}) \delta_{i_0i} \delta_{j_0j} + t_{i_0j_0}^{i'j'} \right] G_{i_0i'j_0j'}^R = \delta_{ii'} \delta_{jj'} + \delta_{j1} \sum_{i_2} \Sigma_{R_{i_2}S_{i_1}} G_{i_2i'1j'}^R + \delta_{jN_y} \sum_{i_2} \Sigma_{R_{i_2}S_{i_1}} G_{i_2i'N_yj'}^R.
\]
3.2 Two-dimensional Nanotransistors

\[ + \delta h \sum_{j'2} \Sigma_{1j'j2}^{RG} G_{1'i'j2}^{R} \]

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 \(N_x \times N_x\)

\[ A \cdot G^{R} = 1. \] (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 \(\Sigma_{RG}^{11} j1\) are set to zero when \(j2 \notin \{j, j \pm 1\}\), 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

\[ A_{jj'}^{ii'} = \begin{cases} 
E - h_{ii'j} - \Sigma_{ii'11}^{RS} \delta_{j1} - \Sigma_{ii'N_yN_y}^{RD} \delta_{jN_y} - \Sigma_{1j'j1}^{RG} \delta_{i1} & i' = i, j' = j \\
\Sigma_{ii'11}^{RS} \delta_{j1} - \Sigma_{ii'N_yN_y}^{RD} \delta_{jN_y} & i' \neq i, j' = j \\
\Sigma_{1j'j1}^{RG} \delta_{i1} & i' = i, j' = j \pm 1 \\
0 & \text{otherwise.}
\end{cases} \] (3.63)

To evaluate the boundary Green’s functions \(\Sigma^{RS}, \Sigma^{RD}, \text{and } \Sigma^{RG}\) 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)

\[ n(x_iy_j) = \frac{1}{2} \Delta_x \Delta_y \sum_{k_z, \sigma} \int \frac{dE}{2\pi} G_{ii'j}^{<}(k_z; E). \] (3.64)

The continuity equation introduced in (2.92) gives

\[ \frac{d}{dt} \rho_{ij}(t) = \lim_{\nu \to t} (-i) e \frac{E}{L_z \Delta_x \Delta_y} \sum_{k_z, \sigma} \left( \frac{d}{dt} G_{ii'j}^{<}(k_z; \nu t') + \frac{d}{dt'} G_{ii'j}^{<}(k_z; \nu t) \right) \]

\[ = - \frac{J_{ij}(t) - J_{i-1j}(t)}{\Delta_x} - \frac{J_{ij}(t) - J_{ij-1}(t)}{\Delta_y}. \] (3.65)
For ballistic transport, the evaluation of equation (3.65) yields
\[
\frac{d}{dt} \rho_{ij}(t) = -\frac{e}{L_z \Delta_x \Delta_y} \sum_{k_z, \sigma} \sum_{i_1j_1} \left( h_{i_1j_1} G_{i_1j_1}^< (k_z; tt) - G_{i_1j_1}^< (k_z; tt) h_{i_1j_1} \right)
\]
(3.66)
and because \( h_{i_1j_1} \) is either diagonal in the \( x \) (\( ii_1 \)) or \( y \) (\( jj_1 \)) direction
\[
\frac{d}{dt} \rho_{ij}(t) = -\frac{e}{L_z \Delta_x \Delta_y} \sum_{k_z, \sigma} \left\{ \sum_{i_1j_1} \left( h_{i_1j_1} G_{i_1j_1}^< (k_z; tt) - G_{i_1j_1}^< (k_z; tt) h_{i_1j_1} \right) + \sum_{j_1} \left( h_{i_1j_1} G_{i_1j_1}^< (k_z; tt) - G_{i_1j_1}^< (k_z; tt) h_{i_1j_1} \right) \right\}
\]
(3.67)
With the ansatz proposed by Caroli in [6], the total current becomes
\[
J_{ij} = -\frac{e}{k L_z} \left( \sum_{i_1 \geq i+1} \sum_{i_2 \leq i} \sum_{k_z, \sigma} \int \frac{dE}{2\pi \Delta_y} \left( h_{i_1j_1} G_{i_1j_1}^< (k_z; E) - G_{i_1j_1}^< (k_z; E) h_{i_1j_1} \right) \right)
\]
(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)
3.3 2D Nanotransistor with Mode Space Method

Figure 3.3: Double Gate Nanotransistor with transverse (z-direction) mode decomposition and 1D solution in x-direction.

which becomes single-dimensional and thus enables the inclusion of rigorous scattering mechanisms. However, this technique only works if the transverse size of the transistor is not too large, otherwise a lot of eigenmodes must be taken into account and one does not gain any size reduction.

A three-dimensional extension of the method seems to be possible but with the same restrictions as mentioned before: the lateral dimensions must remain small.

A detailed description of the model follows with a particular attention on the improvement and drawback compared to the method proposed by A. Svizhenko et al. and presented in the previous section.

3.3.1 Model Summary

The simulated device structure is shown in Figure 3.3, where a uniform rectangular grid with a grid spacing of $\Delta_x$ and $\Delta_z$ is used. The discretization procedure is similar to the one presented in the previous section for the 2D-nanostructure. Only
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 $x_z$ and $z_y$ yields
\[
G_{ij}(z') = \sum_{k_y} \sum_{k_y} \phi_{ij}(xz)G_{ij}(k_y; tt')\phi_{ij}^*(x'z')e^{ik_y(y-y')},
\]
\[
G_{ij}(k_y; tt') = \int dr' \int dr' \phi_{ij}^*(xz)G(11')(x'z')e^{-ik_y(y-y')}. \tag{3.69}
\]
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
\[
(E - H - \Sigma^R) G^< = \Sigma^< G^A
\]
\[
(E - H - \Sigma^R) G^R = I, \tag{3.70}
\]
where $E$ and $I$ are diagonal ($N_x N_z \times N_x N_z$) matrices and $G^<$, $G^R$, $G^A$, $\Sigma^R$,
and $\Sigma^<$ are full ($N_x N_z \times N_x N_z$) matrices. In fact they are composed of $N_x N_z$
submatrices of size $N_x N_z$, each of them representing a slice in the $z$-direction. This
is important when one considers the Hamiltonian matrix $H$ whose elements are
given by
\[
h_{ii'jj'} = \begin{cases}
t_{ii'jj'}^{+1} + t_{ii'jj'}^{-1} + t_{ii'jj'}^{+1} + t_{ii'jj'}^{-1} + V_{ij} + \frac{h^2 k^2}{2m^*} & i' = i, j' = j \\
h_{ii\pm 1jj} = -t_{ii'jj} \pm 1 & i' = i \pm 1, j' = j \\
h_{iijj\pm 1} = -t_{ii'jj} \pm 1 & i' = i, j' = j \pm 1. \\
0 & \text{otherwise.}
\end{cases}
\]
The $t_{ii'jj'}$'s have the following values
\[
t_{ii'jj'}^{\pm 1} = \begin{cases}
\frac{h^2}{(m_t + m_{t\pm 1})} & i' = i \pm 1, j' = j, \\
\frac{h^2}{(m_t + m_{t\pm 1})} & i = i, j' = j \pm 1, \\
0 & \text{otherwise.}
\end{cases} \tag{3.71}
\]
By taking into account all these definitions, the Hamiltonian matrix $H$ can be
written in a simple form, where each element is a $N_x N_z$ submatrix
\[
H = \begin{pmatrix}
\alpha_1 & \beta_{12} & 0 & \cdots & \cdots \\
\beta_{21} & \alpha_2 & \beta_{23} & 0 & \cdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \beta_{N_x-1N_z-2} & \alpha_{N_z-1} & \beta_{N_x-1N_z-1} \\
0 & \cdots & 0 & \beta_{N_xN_z-1} & \alpha_{N_z}
\end{pmatrix}, \tag{3.72}
\]
3.3 2D Nanotransistor with Mode Space Method

\[ \alpha_i = \begin{pmatrix} h_{i11} & h_{i12} & 0 & \cdots & \cdots \\ h_{i12} & h_{i22} & h_{i23} & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & h_{iN_z-1N_z-1} & h_{iN_z-1N_z-1} & h_{iN_zN_z} \\ 0 & \cdots & 0 & h_{iN_zN_z} & h_{iN_zN_z} \end{pmatrix}, \quad (3.73) \]

\[ \beta_{i12} = \begin{pmatrix} h_{i1121} & 0 & \cdots & \cdots & \cdots \\ 0 & h_{i1222} & 0 & \cdots & \cdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & h_{i12N_z-1N_z-1} & 0 & \cdots \\ 0 & \cdots & \ddots & \ddots & h_{i12N_zN_z} \end{pmatrix}, \quad (3.74) \]

The idea behind the mode space expansion of the Green’s functions is the search of the eigenfunctions \( v_{in} \) (size \( N_z \times 1 \)) and eigenenergies \( E_{in} \) of the \( \alpha \)'s matrices \( n \) corresponds to the \( n \)th mode and \( i \) determines it position, i.e. \( x_i \). From the \( N_z \) found eigenfunctions \( v_{in} \), 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 \( (N_zN_m)^2 \times N_k \times N_E \) instead of \( (N_zN_z)^2 \times N_k \times N_E \). These sizes correspond to the number of unknown Green’s functions one is looking for. One has therefore

\[ \alpha_i v_{n}^i = E_{n}^i v_{n}^i \quad (3.75) \]

and the eigenvectors \( v_{n}^i \) are used to build the transformation matrix \( U \) whose size is \( (N_zN_z) \times (N_mN_x) \)

\[ U = \sqrt{\Delta_z} \begin{pmatrix} v_1^1 & \cdots & v_{N_m}^1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & v_1^2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & 0 & \cdots & v_{N_m}^{N_x-1} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 & v_1^{N_x} & \cdots & v_{N_m}^{N_x} \end{pmatrix} \quad (3.76) \]

\( U \) has interesting properties due to the orthogonality of the eigenvectors \( v_{n}^i \): \( U^T \cdot U = I_{N_zN_m \times N_zN_m} \). If one defines now the \( N_z \times N_m \) matrix \( v^i = [v_1^i \ v_2^i \ \cdots \ v_{N_m}^i] \), the notation for the matrix \( U \) can be further simplified and becomes

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

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 $G_{rs}$ in the real space and $G_{ms}$ in the mode space is given by

$$G_{ms} = U^T G_{rs} U, \quad G_{rs} = U G_{ms} U^T.$$  \hspace{1cm} (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 $G_R$ (the same holds for the lesser) on the left with $U^T$ and on the right with $U$, one obtains

$$U^T (E - H - \Sigma^R) G_{rs}^R U = I_{N_m N_x N_m N_x}$$

$$\left( U^T (E - H) U - U^T \Sigma^R U \right) G_{ms}^R = I_{N_m N_x N_m N_x}.$$  \hspace{1cm} (3.79)

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

$$H_{ms} = \begin{pmatrix} E - E^1 & -\gamma_{12} & 0 & \cdots & \cdots \\ -\gamma_{21} & E - E^2 & -\gamma_{23} & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \gamma_{N_x - 1N_x - 2} & E - E^{N_x - 1} & \gamma_{N_x - 1N_x} \\ 0 & \cdots & 0 & \gamma_{N_x - 1N_x - 1} & E - E^{N_x} \end{pmatrix}$$  \hspace{1cm} (3.80)

where

$$E = E \times I_{N_m \times N_m}, \quad E^i = \begin{pmatrix} E_1^i & 0 & \cdots & 0 \\ 0 & E_2^i & \cdots & 0 \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & E_{N_m}^i \end{pmatrix}$$  \hspace{1cm} (3.81)

and

$$\gamma_{ij} = \nu^{jT} \beta_{ij} \nu^i$$  \hspace{1cm} (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 $\beta_{ij}$ 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 $\gamma_{ij}$ submatrices are diagonal. If for simplicity one assumes that $\gamma_{ij}$ 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)

\[
\Sigma_{ii'jj'}(k_y;tt') = \int \! dr \int \! dr' \phi_{ij}^*(xz) \Sigma(11') \phi_{ij'}(x'z') e^{-ik_y(y-y')}
\]

(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 \(v_{i'n}(z)\) coming from the submatrix \(\alpha_i\) situated at \(x_i\). This yields the following expression

\[
\Sigma_{ii'm'n'}(k_y;tt') = \int \! dr \int \! dr' \phi_{i'}^*(x)v_{im}^*(z) \Sigma(11')v_{n'm'}^*(z') \phi_{i'}(x') e^{-ik_y(y-y')}
\]

(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 \((N_xN_m) \times (N_yN_m)\) 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 \(\gamma_{ij}\) 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 Quantum Cascade Structures

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, $H = H_0 + H_{\text{scatt}}$, where $H_0 = H_{\text{SL}} + H_{\text{E}}$ is treated exactly and $H_{\text{scatt}}$ as perturbation through self-energies. $H_{\text{SL}}$ models the superlattice potential while $H_{\text{E}} = -eEz$ describes the effects of the electric field $E$ applied in the growth direction.

3.4.1.1 Bloch States

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

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

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

$$\psi^\nu_k(r, z + d) = e^{jqd} \psi^\nu_k(r, z),$$

where $q$ takes values between $-\frac{\pi}{d}$ and $\frac{\pi}{d}$. This implies that the energy $E^\nu(k, q)$ and the wave function $\psi^\nu_{k,q}(r, z) = \frac{e^{jkx}}{\sqrt{A}} \phi^\nu_q(z)$ 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

$$E^\nu(k, q) = E^\nu + \sum_{h=1}^{\infty} 2T^\nu_h \cos(hdq) + \frac{\hbar^2 k^2}{2m^*}.$$  \hspace{1cm} (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 $\hat{\psi}^\dagger(r,t)$ and annihilation $\hat{\psi}(r,t)$ operators, which will be given by

$$\hat{\psi}^\dagger(r,t) = \sum_{\nu,k} \int dq \frac{e^{-jk \cdot r}}{\sqrt{A}} \phi^\nu_q(z) a^\nu_{k,q}(t)$$

$$\hat{\psi}(r,t) = \sum_{\nu,k} \int dq \frac{e^{jk \cdot r}}{\sqrt{A}} \phi^\nu_q(z) a^\nu_{k,q}(t).$$  \hspace{1cm} (3.87)
wave functions are changed from Bloch the operators \(a_{k,q}^{-}\) and \(a_{k,q}^{+}\), respectively. Furthermore, one has the property

\[
\int dz \phi_{q_1}^{\nu_1}(z) \phi_{q_2}^{\nu_2}(z) = \delta_{\nu_1,\nu_2} \delta(q_1 - q_2).
\]

(3.88)

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

\[
G(11') = -\frac{i}{\hbar} \langle \hat{\psi}(r, t) \hat{\psi}^\dagger(r', t') \rangle
\]

\[
= \frac{1}{A} \sum_{\nu_1, \nu_2, k} \int dq_1 \int dq_2 \phi_{q_1}^{\nu_1}(z) \left( -\frac{i}{\hbar} \langle T \left\{ \phi_{k,q_1}^{\nu_1}(t) \phi_{k,q_2}^{\nu_2}(t') \right\} \phi_{q_2}^{\nu_2}(z') e^{i k (r_1 - r_2)} \right)
\]

\[
= \frac{1}{A} \sum_{\nu_1, \nu_2, k} \int dq_1 \int dq_2 \phi_{q_1}^{\nu_1}(z) G_{\nu_1 \nu_2}(k \delta_{q_1 q_2}; tt') \phi_{q_2}^{\nu_2}(z') e^{i k (r_1 - r_2)}.
\]

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 \(M_{n,n_1}\) 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

\[
\psi^{\nu}(z - nd) = \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} dq e^{-inqd} \phi_{q}^{\nu}(z)
\]

\[
\phi_{q}^{\nu}(z) = \sqrt{\frac{d}{2\pi}} \sum_{n} e^{inqd} \psi^{\nu}(z - nd)
\]

(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

\[
\int dz \psi^{\nu_1}(z - nd) \psi^{\nu_2}(z - md) = \delta_{\nu_1,\nu_2} \delta_{nm}.
\]

(3.90)

\(\psi^{\nu}(z - nd)\) is associated with miniband \(\nu\) 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 \(a_{k,q}^{\nu} \) and \(a_{k,q}^{\nu\dagger}\) must also be modified, in order that the position and time
dependent annihilation and creation operators  \( \hat{\psi}(r, t) \) and  \( \hat{\psi}^\dagger(r, t) \) remain constant. For instance,  \( \psi(r, t) \) must destroy an electron at place  \( r \) and time  \( t \)

\[
\hat{\psi}(r, t) = \sum_{\nu,k} \int \frac{d^3k}{\sqrt{A}} \phi_{q}^\nu(z) a_{k,q}^\nu(t)
\]

\[
= \sum_{\nu,k} \sum_n e^{j k_{xy}} \psi^\nu(z - nd)a_{k,n}^\nu(t)
\]

\[
\Rightarrow a_{k,n}^\nu = \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} dq \ e^{j n q d} a_{k,q}^\nu
\]

\[
a_{k,q}^\nu = \sqrt{\frac{d}{2\pi}} \sum_n e^{-j n q d} a_{k,n}^\nu
\]

(3.91)

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

\[
G(11') = \frac{i}{\hbar} \langle \hat{\psi}(r, t) \hat{\psi}^\dagger(r', t') \rangle
\]

\[
= \frac{1}{A} \sum_{\nu_1, \nu_2: \pm} \sum_{k, nm} \psi^{\nu_1}(z - nd) \left( -\frac{i}{\hbar} \right) \langle \hat{a}_{k,n}^{\nu_1}(t) \hat{a}_{k,m}^{\nu_2}(t') \rangle \psi^{\nu_2}(z' - md) e^{i k (r_{xy} - r'_{xy})}
\]

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

\[
h_{nm}^{\nu_1 \nu_2} = \int dz \ \psi^{\nu_1\star}(z - nd) H_0 \psi^{\nu_2}(z - md)
\]

\[
= \int dz \ \psi^{\nu_1\star}(z - nd) H_{SL} \psi^{\nu_2}(z - md)
\]

\[
+ \int dz \ \psi^{\nu_1\star}(z - nd) H_{E} \psi^{\nu_2}(z - md)
\]

\[
H_{SLnm}^{\nu_1 \nu_2} = H_{SLnm}^{\nu_1 \nu_2} + H_{Enm}^{\nu_1 \nu_2}
\]

\[
H_{SLnm}^{\nu_1 \nu_2} = \frac{d}{2\pi} \int dq_1 \int dq_2 \int dz \ \phi_{q_{1}}^{\nu_1}(z) H_{SL} \phi_{q_{2}}^{\nu_2}(z) e^{j n q d} e^{-j m q d}
\]

\[
= \frac{d}{2\pi} \int dq_1 \int dq_2 \ \delta_{\nu_1, \nu_2} \delta(q_1 - q_2) e^{j (n - m) q d}
\]

\[
= \delta_{\nu_1, \nu_2} \cdot \left\{ \begin{array}{ll}
E_{H}^{\nu_1} & m = n,
T_{H}^{\nu_1} & m = n \pm h,
\end{array} \right. h \geq 1
\]
Green's functions becomes simplifies the matrix equation (3.93). For example, the equation for the retarded conduction-band offset and one above (the indices following example: a superlattice structure has nine different minibands below the
tions). Hence one can assume that \( \Sigma \) diagonalized, and the resulting eigenfunctions give the required set of Wannier operator \( \hat{\Sigma} \) and the Hamiltonian \( \hat{H} \) is explained in [15] (the position superlattice period, so that the overlap integrals, and therefore the self-energies \( \Sigma \) the advantage of the Wannier functions is that they are localized, in this case over a

diagonalized 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

\[
E G_{nm}^{<\nu_1\nu_2}(k_t; E) - \sum_{l\nu_3} h_{nl}^{\nu_1\nu_3} G_{lm}^{<\nu_1\nu_2}(k_t; E) = \sum_{l\nu_3} \sum_{l\nu_3}^{R\nu_1\nu_3}(k_t; E) E G_{lm}^{<\nu_1\nu_2}(k_t; E) + \sum_{l\nu_3}^{<\nu_1\nu_2}(k_t; E) E G_{lm}^{>\nu_1\nu_2}(k_t; E)
\]

\[
E G_{nm}^{R\nu_1\nu_2}(k_t; E) - \sum_{l\nu_3} h_{nl}^{\nu_1\nu_3} G_{lm}^{R\nu_1\nu_2}(k_t; E) = \delta_{nm}\delta_{\nu_1\nu_2} + \sum_{l\nu_3} h_{nl}^{\nu_1\nu_3} G_{lm}^{R\nu_1\nu_2}(k_t; E) G_{lm}^{R\nu_1\nu_2}(k_t; E).
\]

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

\[
G_{nm}^{\nu_1\nu_2}(k; E) = G_{n-1m-1}^{\nu_1\nu_2}(k; E + e\mathcal{E}d).
\]

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 \( \nu \) run therefore from 1 to 10).
3.4 Quantum Cascade Structures

The Green’s functions of one period are only coupled to themselves, and the Green’s functions of the 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

\[
n(z) = -\frac{i}{4} \sum_{k_\sigma} \sum_{n \nu_1 \nu_2} \sum_{m \nu_1 \nu_2} \int \frac{dE}{2\pi} G_{nm}^{<\nu_1 \nu_2}(k; E) \psi_{\nu_1}^\dagger(z - nd) \psi_{\nu_2}^\dagger(z - md).
\]  

(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

\[
J = \frac{e}{V} \langle \hat{v} \rangle = \frac{e}{V} \left\langle \frac{d}{dt} \hat{z} \right\rangle
\]  

(3.96)

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

\[
\hat{z} = \sum_{nm \nu_1 \nu_2} \sum_{k_\sigma} \sum_{\nu_1 \nu_2} \nu_{nm}^{\nu_1 \nu_2} a_{k,n}^{\nu_1} a_{k,m}^{\nu_2} = \sum_{nm \nu_1 \nu_2} \sum_{k_\sigma} \sum_{\nu_1 \nu_2} \int dz \psi_{\nu_1}^\dagger(z - nd) \psi_{\nu_2}^\dagger(z - md) a_{k,n}^{\nu_1} a_{k,m}^{\nu_2}.
\]  

(3.97)

The current density can then be written as

\[
J = -ie \int \frac{dE}{V} \sum_{n \nu_1 \nu_2} \sum_{k_\sigma} \sum_{\nu_1 \nu_2} \nu_{nm}^{\nu_1 \nu_2} \lim_{t' \to t} \left( \frac{d}{dt} + \frac{d}{dt'} \right) G_{nm}^{\nu_1 \nu_2}(k; t)
\]  

\[
= -\frac{e}{V} \sum_{nm \nu_1 \nu_2} \sum_{k_\sigma} \sum_{\nu_1 \nu_2} \nu_{nm}^{\nu_1 \nu_2} \left\{ \left( t_m^{\nu_2 \nu_3} G_{lm}^{<\nu_1 \nu_1}(k; t) + G_{ml}^{<\nu_2 \nu_2}(k; t) \right) h_{ln}^{\nu_1 \nu_1} \right\} + \int dt_2 \left[ \left( t_m^{R \nu_2 \nu_3}(k; t_2) G_{lm}^{<\nu_1 \nu_1}(k; t) + \Sigma_{ml}^{\nu_2 \nu_2}(t_2) G_{ln}^{A \nu_1 \nu_1}(k; t_2) \right) - \left[ G_{ml}^{R \nu_2 \nu_3}(k; t_2) \Sigma_{lm}^{\nu_1 \nu_1}(k; t_2) + \Sigma_{ml}^{\nu_2 \nu_2}(k; t_2) G_{ln}^{A \nu_1 \nu_1}(k; t_2) \right] \right)
\]  

\[
= -\frac{e}{\hbar V} \sum_{nm \nu_1 \nu_2} \sum_{k_\sigma} \sum_{\nu_1 \nu_2} \int \frac{dE}{2\pi} \left\{ \left( \nu_{nm}^{\nu_1 \nu_2} h_{ml}^{\nu_1 \nu_2} - h_{nm}^{\nu_1 \nu_2} \nu_{ml}^{\nu_1 \nu_2} \right) G_{ln}^{<\nu_1 \nu_1}(k; E) + \nu_{nm}^{\nu_1 \nu_2} \left( t_m^{R \nu_2 \nu_3}(k; E) G_{ln}^{<\nu_1 \nu_1}(k; E) + \Sigma_{ml}^{\nu_2 \nu_2}(k; E) G_{ln}^{A \nu_1 \nu_1}(k; E) \right) \right) - \right.
\]
\begin{equation}
Z_{nm}^{\nu_1 \nu_2} \left\{ G_{ml}^{R \nu_2 \nu_3} (k_l; E) \Sigma_{in}^{< \nu_1 \nu_3} (k_l; E) + G_{ml}^{< \nu_2 \nu_3} (k_l; E) \Sigma_{in}^{> \nu_1 \nu_3} (k_l; E) \right\}.
\end{equation}

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 \( H_{\text{scatt}}, J_{\text{scatt}} \) 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 \( k_l \) must be accomplished. This summation is transformed into an integral over an angle \( \theta \) and over the norm \( k \) of the wave vector. To simplify the numeric, the terms which should be integrated over the angle \( \theta \) 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

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

with the formal solution

$$|\Psi_S(t)\rangle = e^{-iH_0t/\hbar} |\Psi_S(0)\rangle = e^{-iH_0t/\hbar} |\Psi_0\rangle. \quad (A.2)$$

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

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

because

$$\frac{d}{dt} |\Psi_H(t)\rangle = \frac{i}{\hbar} [H e^{iHt/\hbar} |\Psi_S(t)\rangle + e^{iHt/\hbar} \frac{d}{dt} |\Psi_S(t)\rangle] = 0. \quad (A.4)$$
In order to get the same matrix elements as in the Schrödinger representation, the Heisenberg operators are defined as follows

\[ O_H(t) = e^{iHt/\hbar} O_S e^{-iHt/\hbar} \]  
\[(A.5)\]

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

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

### 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

\[ |\Psi_I(t)\rangle = e^{iH_0t/\hbar} |\Psi_S(t)\rangle \]
\[ = e^{iH_0t/\hbar} e^{-iHt/\hbar} |\Psi_0\rangle \]
\[ = U_I(t) |\Psi_0\rangle \]  
\[(A.7)\]

for the wave function and

\[ O_I(t) = e^{iH_0t/\hbar} O_S e^{-iH_0t/\hbar} \]  
\[(A.8)\]

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

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

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

\[ i\hbar \frac{d}{dt} |\Psi_I(t)\rangle = V_I(t) |\Psi_I(t)\rangle \]  
\[(A.10)\]

and of the development operator \( U_I(t) = e^{iH_0t/\hbar} e^{-iHt/\hbar} \) with \( U_I(0) = 1 \), which obeys the following differential equation

\[ i\hbar \frac{d}{dt} U_I(t) = V_I(t) U_I(t). \]  
\[(A.11)\]

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

\[ U_I(t) - U_I(0) = -\frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) U_I(t_1) \]  
\[(A.12)\]
or

\[
U_I(t) = 1 - \frac{i}{\hbar} \int_0^t dt_1 V_I(t_1)U_I(t_1).
\]  

(A.13)

If this equation is repeatedly iterated, one gets

\[
U_I(t) = 1 - \frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) + \left( -\frac{i}{\hbar} \right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V_I(t_1)V_I(t_2) + \ldots + \left( -\frac{i}{\hbar} \right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n V_I(t_1)V_I(t_2) \ldots V_I(t_n) \\
= \sum_{n=0}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n V_I(t_1)V_I(t_2) \ldots V_I(t_n).
\]

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]:

\[
U_I(t) = 1 + \sum_{n=1}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_0^t dt_1 \int_0^t dt_2 \ldots \int_0^t dt_n T^c \{ V_I(t_1)V_I(t_2) \ldots V_I(t_n) \} \\
= T^c \{ \exp \left( -\frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) \right) \}.
\]  

(A.14)

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

\[
-i\hbar \frac{d}{dt} U_I^{-1}(t) = U_I^{-1}(t)V_I(t)
\]  

(A.15)

with the solution

\[
U_I^{-1}(t) = 1 + \sum_{n=1}^{\infty} \left( \frac{i}{\hbar} \right)^n \int_0^t dt_1 \int_0^t dt_2 \ldots \int_0^t dt_n T^n \{ V_I(t_1)V_I(t_2) \ldots V_I(t_n) \} \\
= T^n \{ \exp \left( \frac{i}{\hbar} \int_0^t dt_1 V_I(t_1) \right) \} \\
= U_I^t(t).
\]  

(A.16)

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

\[
T^n \{ A(t)B(t') \} = \theta(t-t')B(t')A(t) + \theta(t'-t)A(t)B(t'),
\]  

(A.17)

but if they are Fermion field operators

\[
T^n \{ A(t)B(t') \} = \theta(t-t')B(t')A(t) - \theta(t'-t)A(t)B(t').
\]  

(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

\[
|\Psi_I(t)\rangle = S(t, t')|\Psi_I(t')\rangle = U_I(t)U_I^\dagger(t')|\Psi_I(t')\rangle
\]

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,

\[
i\hbar \frac{d}{dt} S(t, t') = V_I(t)S(t, t')
\]

which has the solution

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

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

\[
\langle O_H(t) \rangle = \langle e^{iH_I t/\hbar} O_I e^{-iH_I t'/\hbar} \rangle
\]

\[
= \langle e^{iH_I t/\hbar} e^{-iH_I t'/\hbar} O_I(t) e^{iH_I t'/\hbar} e^{-iH_I t/\hbar} \rangle. \tag{A.22}
\]

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

\[
\langle O_H(t) \rangle = \langle U_I^\dagger(t)O_I(t)U_I(t) \rangle
\]

\[
= \langle S^\dagger(t, 0)O_I(t)S(t, 0) \rangle
\]

\[
= \langle S(0, t)O_I(t)S(t, 0) \rangle. \tag{A.23}
\]

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

\[
\langle O_H(t) \rangle = \langle S(t_o, t)O_I(t)S(t, t_o) \rangle. \tag{A.24}
\]

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 $\rho$ present in the thermodynamic average of equation (1.10) for example

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

The density operator $\rho_S$ obeys the following differential equation

$$\frac{d\rho_S}{d\beta} = -(H - \mu N)\rho_S.$$  \hspace{1cm} (B.2)

B.2 Pseudo Heisenberg Picture

The pseudo Heisenberg density operator $\rho_H$ is given by:

$$\rho_H = e^{\beta(H-\mu N)}\rho_S$$ \hspace{1cm} (B.3)

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

$$O_H(\tau) = e^{\tau(H-\mu N)/\hbar}O_Se^{-\tau(H-\mu N)/\hbar}.$$ \hspace{1cm} (B.4)

B.3 Pseudo Interaction Picture

In this representation, the density operator $\rho_I$ is given by

$$\rho_I = e^{\beta(H_0-\mu N)}\rho_S = e^{\beta(H_0-\mu N)}e^{\beta(H-\mu N)}.$$ \hspace{1cm} (B.5)
and the operators in the pseudo-interaction picture obey the following equation
\[ O_I(\tau) = e^{\tau(H_0 - \mu N)/\hbar} O_S e^{-\tau(H_0 - \mu N)/\hbar}. \]  

(B.6)

To recall a formalism similar to the one described in Appendix A, a time development operator \( \mathcal{U}(\tau) \) is introduced with
\[ \mathcal{U}(\tau) = \rho_I \left( \beta - \frac{\tau}{\hbar} \right). \]  

(B.7)

Then, \( \mathcal{U}(\tau) \) is governed by a differential equation very similar to (A.11)
\[ \frac{d}{d\tau} \mathcal{U}_I(\tau) = V_I(\tau) \mathcal{U}_I(\tau). \]  

(B.8)

Integrating both sides of the equation with respect to the imaginary time \( \tau \) yields
\[ \mathcal{U}_I(\tau) - \mathcal{U}_I(0) = -\frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \mathcal{U}_I(\tau_1) \]  

(B.9)
or
\[ \mathcal{U}_I(\tau) = 1 - \frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \mathcal{U}_I(\tau_1). \]  

(B.10)

If this equation is repeatedly iterated, one obtains
\[ \mathcal{U}_I(\tau) = 1 - \frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) + \left( -\frac{1}{\hbar} \right)^2 \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n) \]
\[ = \sum_{n=0}^{\infty} \left( -\frac{1}{\hbar} \right)^n \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n). \]

With the help of the imaginary time-order operator \( T_\tau \), the expression for \( \mathcal{U}_I(\tau) \) can be simplified [5]
\[ \mathcal{U}_I(\tau) = 1 + \sum_{n=1}^{\infty} \left( -\frac{1}{n!} \right)^n \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 \cdots \int_0^\tau d\tau_n T_\tau \{ V_I(\tau_1) V_I(\tau_2) \cdots V_I(\tau_n) \} \]
\[ = T_\tau \{ \exp \left( -\frac{1}{\hbar} \int_0^\tau d\tau_1 V_I(\tau_1) \right) \}. \]  

(B.11)

### B.3.1 S Matrix

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

- \( S(\tau, \tau) = 1 \)
- \( S(\tau, \tau') S(\tau', \tau'') = S(\tau, \tau'') \)
• $S(\tau, \tau')$ can be expressed as a time-ordered operator,

$$\hbar \frac{d}{d\tau} S(\tau, \tau') = V_I(\tau) S(\tau, \tau')$$  \hspace{1cm} \text{(B.12)}

which has the solution

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

External Perturbation

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

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

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

$$i\hbar \frac{d}{dt} |\psi_S(t)\rangle = \mathcal{H}(t) |\psi_S(t)\rangle = \left( H + H^{\text{ext}}(t) \right) |\psi_S(t)\rangle.$$  \hspace{1cm} (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

$$i\hbar \frac{d}{dt} U_S(t, t_0) = \mathcal{H}(t) U_S(t, t_0).$$  \hspace{1cm} (C.3)

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

$$U_S(t, t_0) = e^{-i \mathcal{H}(t-t_0)/\hbar} S_H^{\text{ext}}(t, t_0).$$  \hspace{1cm} (C.4)

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

$$i\hbar \frac{d}{dt} S_H^{\text{ext}}(t, t_0) = e^{i \mathcal{H}(t-t_0)/\hbar} H^{\text{ext}}(t) e^{-i \mathcal{H}(t-t_0)/\hbar} S_H^{\text{ext}}(t, t_0) = H^{\text{ext}}(t) S_H^{\text{ext}}(t, t_0).$$  \hspace{1cm} (C.5)

The solution is obtained by repeated iteration of the equation

$$S_H^{\text{ext}}(t, t_0) = T \left\{ \exp \left( -i \int_{t_0}^{t} dt_1 H^{\text{ext}}(t_1) \right) \right\}.$$  \hspace{1cm} (C.6)

As $t_o$ is the initial time of the system, $t$ is always larger than $t_o$ and the time operator $T$ corresponds to the chronological time-ordering operator $T_c$. $S_H^{\text{ext}}(t, t_0)$ has the same properties as the $S$ matrix introduced in Appendix A.
C.1 Heisenberg Representation

A wave function $|\psi_H(t)\rangle$ and an operator $O_H(t)$ in the Heisenberg representation with respect to $H$ are introduced

$$|\psi_H(t)\rangle = U_{S}^{-1}(t,t_0)|\psi_S(t)\rangle$$
$$O_H(t) = U_{S}^{-1}(t,t_0)O_S U_S(t,t_0).$$

(C.7)

Therefore, one obtains for the expectation value $\langle O_H(t) \rangle$

$$\langle O_H(t) \rangle = \langle U_{S}^{-1}(t,t_0)O_S U_S(t,t_0) \rangle = \langle S_{H}^{ext}(t,t_0)e^{iH(t-t_0)}\rangle O_S e^{-iH(t-t_0)/\hbar} S_{H}^{ext}(t,t_0)$$
$$= \langle S_{H}^{ext}(t,t_0)O_H(t)S_{H}^{ext}(t,t_0) \rangle.$$  

(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 $H(t)$ are defined by

$$G(x,t; x',t') = -\frac{i}{\hbar} \langle \psi_H(x,t) \hat{\psi}_H^\dagger(x',t') \rangle.$$  

(C.9)

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

$$G(x,t; x',t') = -\frac{i}{\hbar} \langle T \left\{ S(t_0,t) \hat{\psi}_H(x,t)S(t,t_0)S(t_0,t')\hat{\psi}_H^\dagger(x',t')S(t',t_0) \right\} \rangle$$
$$= -\frac{i}{\hbar} \langle T \left\{ S(t_0,t) \hat{\psi}_H(x,t)S(t,t')\hat{\psi}_H^\dagger(x',t')S(t',t_0) \right\} \rangle \langle S(t_0,t_0) \rangle$$
$$= -\frac{i}{\hbar} \langle T \left\{ S_{H}^{ext}(t_0,t_0)\hat{\psi}_H(x,t)\hat{\psi}_H^\dagger(x',t') \right\} \rangle \langle S_{H}^{ext}(t_0,t_0) \rangle$$

(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

$$S_{H}^{ext}(t_0,t_0) = T \left\{ \exp \left( -\frac{i}{\hbar} \int_{t_0}^{t_0} dt_1 H_{H}^{ext}(t_1) \right) \right\}.$$  

(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

\[
\langle O \rangle = \frac{\text{Tr}(\rho O)}{\text{Tr}(\rho)}
\]

• the density operator \( \rho \) must be of the form

\[
\rho = \exp(A)
\]  

with \( A \) being a 1-particle operator like \( A = \sum A_j c_j^\dagger c_j \). 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).

\[
\langle T\{A_I B_I \cdots Y_I Z_I \} \rangle = A_I B_I \cdots Y_I Z_I + A_I B_I \cdots Y_I Z_I + \cdots
\]

= sum over all possible contracted products  

where the contraction

\[
A_I^* B_I = \langle T\{A_I B_I \} \rangle
\]

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

\[
A_I(x_1, t_1)B_I(x_2, t_2) = i\hbar G_0(x_1, t_1; x_2, t_2) \tag{D.4}
\]

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

\[
A_I(x_1, t_1)B_I(x_2, t_2) = i\hbar G_0(x_2, t_2; x_1, t_1). \tag{D.5}
\]

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

\[
V = \frac{1}{2} \int dx_1 \int dx_2 \hat{\psi}_I^\dagger(x_1) \hat{\psi}_I(x_2) V(x_1 - x_2) \hat{\psi}(x_2) \hat{\psi}(x_1). \tag{D.6}
\]

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

\[
F^{(0)}_N = \langle T\{\hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle = i\hbar G_0(x, t; x', t'). \tag{D.7}
\]

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

\[
F^{(1)}_N = \langle T\{-\frac{i}{\hbar} \int dt_1 V_I(t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle
\]

\[
= -\frac{i}{\hbar} \frac{1}{2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \cdot \langle T\{\hat{\psi}_I^\dagger(x_1, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x_2, t_1) \hat{\psi}_I(x, t) \hat{\psi}_I^\dagger(x', t') \} \rangle. \tag{D.8}
\]

There are six non-vanishing possibilities to contract equation (D.8) with the Wick’s theorem
body problems and illustrate the perturbation expansion of the Green’s functions. 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.

\[ F_N^{(1)} = -\frac{i}{\hbar^2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \]

\[ \times \left[ \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_1, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_1, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_1, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x_1, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') + \psi^\dagger(x_1, t_1) \psi^\dagger(x_2, t_1) \psi^\dagger(x, t) \psi^\dagger(x', t') \right] \quad \text{(D.9)} \]

Replacing the contraction products by free Green’s functions \(G_0\) (no \(i\) for the Matsubara Green’s functions),

\[ F_N^{(1)} = -\frac{i}{\hbar^2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \]

\[ \times \left[ -i \hbar G_0(x_2, t_1; x_1, t_1^+) (i \hbar G_0(x_1, t_1; x_2, t_1^+) i \hbar G_0(x, t; x', t') - i \hbar G_0(x, t; x_2, t_1) i \hbar G_0(x_1, t_1; x', t')) \right. \]

\[ + i \hbar G_0(x_1, t_1; x_1, t_1^+) (i \hbar G_0(x_2, t_1; x_2, t_1^+) i \hbar G_0(x, t; x', t') - i \hbar G_0(x, t; x_2, t_1) i \hbar G_0(x_2, t_1; x', t')) \]

\[ + i \hbar G_0(x, t; x_2, t_1) (i \hbar G_0(x_1, t_1; x_2, t_1^+) i \hbar G_0(x, t_1; x', t') - i \hbar G_0(x_2, t_1; x_2, t_1^+) i \hbar G_0(x, t_1; x', t')) \left. \right] \quad \text{(D.10)} \]

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:

\[ F_D^{(1)} = -\frac{i}{\hbar^2} \int dt_1 \int dx_1 \int dx_2 V(x_1 - x_2) \]

\[ \times \left[ -i \hbar G_0(x_2, t_1; x_1, t_1^+) i \hbar G_0(x_1, t_1; x_2, t_1^+) \right. \]

\[ + i \hbar G_0(x_1, t_1; x_1, t_1^+) i \hbar G_0(x, t_1; x_2, t_1^+) \left. \right] \quad \text{(D.10)} \]

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 \(n = 1, 2, \cdots, \infty\). 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

\[
G(x_t; x'_t') = \frac{-i}{\hbar} \langle \hat{\psi}_H(x, t) \hat{\psi}^\dagger(x', t') \rangle \tag{E.1}
\]

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

\[
(x', t') \quad \text{---} \quad (x, t) \tag{E.2}
\]

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

\[
(x', t') \quad \text{via} \quad \frac{i}{\hbar} G_0(xt; x't') \quad (x, t).
\]  

(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)

\[
\text{or } \quad (x_1 \rightarrow x_2).
\]  

(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

\[
\text{or } \quad \text{or}
\]  

(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 \( \omega \), 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

\[
(x', t') \quad \text{via} \quad (x_1, t_1) \quad (x, t) \quad \Rightarrow \quad \int dt_1 \int dx_1.
\]  

(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 \((k, \omega)\)-space than in the \((x, t)\)-space. A free phonon and the interaction between carriers and phonons are represented by

\[
\begin{align*}
\text{and } -i\frac{q}{\hbar} \quad (\text{E.7})
\end{align*}
\]

\[
\begin{align*}
\text{E.2 Simple Application}
\end{align*}
\]

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

\[
G(x, t; x', t') = G^{(0)}(x, t; x', t') + G^{(1)}(x, t; x', t') + G^{(2)}(x, t; x', t') + \cdots \tag{E.8}
\]

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 \(G^{(0)}(x; t; x'; t')\) is obviously the free Green’s function described by the Feynman diagram E.3. For the first order perturbation \(G^{(1)}(x; t; x'; t')\), 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.

\[
i\hbar G_N^{(1)}(x; t; x'; t') = \]

\[
\begin{align*}
(x_1 t_1) @ (x_2 t_1) + (x' t') \quad (x t) + (x' t') \quad (x_1 t_1) \quad (x_2 t_1) \quad (x t)
\end{align*}
\]

\[
\begin{align*}
(x_1 t_1) @ (x_2 t_1) + (x' t') \quad (x t) + (x' t') \quad (x_2 t_1) \quad (x t)
\end{align*}
\]
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 \(G_N^{(2)}(x t; x' t')\) or \(G_N^{(3)}(x t; x' t')\) 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

\[
\begin{align*}
(x_1 t_1) & \quad \otimes \quad (x_2 t_1) \\
(x' t') & \quad \otimes \quad (x_3 t_3) (x_4 t_3)
\end{align*}
\]

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 \(G^{(1)}(x, t; x', t')\)

\[
i h G^{(1)}(x, t; x', t') = \quad \text{+}
\]
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 $\frac{V_I V_I}{2}$ factors. This yields for these two terms

$$i\hbar G^{(2)}(x, t; x', t') = \frac{1}{A_3} (x't') (xt) + \frac{1}{A_4} (x't') (xt).$$

### 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

![Diagrams](image)

(E.10)

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 cannot 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 $\Sigma$. With the first order and the two most important diagrams of second order, one gets for the self-energy $\Sigma$

$$\Sigma = \frac{i}{\hbar} \Sigma(x_1, t_1; x_2, t_2)$$

(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

\[ + \left( \begin{array}{c}
\vdots \\
\end{array} \right) = \]

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 \( \Sigma \) the following self-consistent equation

\[ \Sigma = \left( \begin{array}{c}
\vdots \\
\end{array} \right) = \]

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

\[ i\hbar G(x,t;x',t') = \left( \begin{array}{c}
\vdots \\
\end{array} \right) + \left( \begin{array}{c}
\vdots \\
\end{array} \right)^2 + \left( \begin{array}{c}
\vdots \\
\end{array} \right)^3 + \cdots \]

Converting the Feynman diagrams into mathematical expressions yields

\[ G(11') = G_0(11') + \int d2 \int d3 \, G_0(12)\Sigma(23)G(31') \]

or

\[ = G_0(11') + \int d2 \int d3 \, G(12)\Sigma(23)G_0(31') \] (E.13)

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

\[-\frac{i}{\hbar} W(12) = \quad \begin{array}{c}
\includegraphics{diagram1}
\end{array} + \begin{array}{c}
\includegraphics{diagram2}
\end{array} + \begin{array}{c}
\includegraphics{diagram3}
\end{array} + \begin{array}{c}
\includegraphics{diagram4}
\end{array} + \cdots \]

Keeping only the Feynman diagrams which are combinations of the bubble diagram \( \includegraphics{bubble} \) preceded and followed by the interaction \( \includegraphics{interaction} \), one gets the screened interaction within the \( \text{RPA} \) (Random Phase Approximation)

\[-\frac{i}{\hbar} W_{\text{RPA}}(12) = \quad \begin{array}{c}
\includegraphics{diagram5}
\end{array} + \begin{array}{c}
\includegraphics{diagram6}
\end{array} + \begin{array}{c}
\includegraphics{diagram7}
\end{array} + \begin{array}{c}
\includegraphics{diagram8}
\end{array} + \cdots \]

Converting the Feynman diagrams into mathematical expressions gives the following equation for the screened interaction within RPA

\[ W_{\text{RPA}}(12) = V(1 - 2) - i\hbar \int d3 \int d4 \, V(1 - 3) G(34) G(43) W_{\text{RPA}}(42) \]

\[ = V(1 - 2) + \int d3 \int d4 \, V(1 - 3) \pi(34) W_{\text{RPA}}(42) \]

(E.14)
\[ V(1 - 2) = V(|x_1 - x_2|) \delta(t_1 t_2) \]  
(E.15)

and

\[ \pi(12) = -i\hbar G(12)G(21) \]  
(E.16)

As consequence, one obtains a direct relation between the bubble diagram and the factor \( \pi(12) \) in the RPA approximation.

\[ i\hbar \pi(12) = \]  
(E.17)

Special care must be taken to include the screened potential \( W(12) \) into equation (E.11) for the self-energy \( \Sigma \). 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)

\[ = \]  
(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

\[ = \]  
(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
In the exchange collision term, screening occurs for all the interactions $V$

$$\Sigma(12) = -\kappa^2 \int d3 \int d4 \ W(13)G(14)G(43)G(32)W(42).$$  
(E.21)

### E.5 Carrier-Phonon Example

Another important many-body effects is the carrier-phonon interaction as described by equation (E.7). One notices the equivalence between carrier-carrier and carrier-phonon Feynman diagrams: for each carrier-carrier diagram, one can find a carrier-phonon diagram where the interaction line is replaced by a phonon line including the carrier-phonon interaction at both extremities. For example, for the two parent diagrams below, one can extract the Green’s function and replace the sum of the carrier-carrier and the carrier-phonon interactions by a zigzag line:

Therefore, the self energy containing both carrier-carrier and carrier-phonon interactions can be rewritten as the following self-consistent equation:

$$\Sigma = \sum + \sum + \sum + \sum + \cdots$$
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:

$$-\frac{i}{\hbar} W_{eff}(12) = \text{zigzag line} = \text{carrier-carrier interaction} + \text{carrier-phonon interaction}$$

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

$$-\frac{i}{\hbar} W^{ph}(12) = -\frac{i}{\hbar} (W_{eff} - W)(12) = \left( \text{zigzag line} + \text{carrier-carrier interaction} \right) - \left( \text{carrier-phonon interaction} \right)$$

To solve this diagram equation, the transformation into the $(k, \omega)$ space provides great advantages, because the equation for $W^{ph}(12)$ can be simplified. Fourier transforming space and time gives

$$-\frac{i}{\hbar} W^{ph}(k\omega) = \frac{\text{zigzag line}}{1 - \text{zigzag line}} - \frac{\text{carrier-phonon interaction}}{1 - \text{carrier-phonon interaction}}$$

$$= \frac{\left( \text{carrier-phonon interaction} + \text{carrier-carrier interaction} \right) \left( 1 - \text{carrier-phonon interaction} \right) - \text{carrier-phonon interaction} \left( 1 - \text{carrier-phonon interaction} - \text{carrier-carrier interaction} \right)}{\left( 1 - \text{carrier-phonon interaction} \right) \left( 1 - \text{carrier-phonon interaction} \right)}$$

$$= \frac{\text{carrier-phonon interaction}}{\left( 1 - \text{carrier-phonon interaction} \right) \left( 1 - \text{carrier-phonon interaction} \right)} = \frac{\text{carrier-phonon interaction}}{\left( 1 - \text{carrier-phonon interaction} \right) \left( 1 - \text{carrier-phonon interaction} \right)}$$

$$= \frac{\text{carrier-phonon interaction}}{\left( 1 - \text{carrier-phonon interaction} \right) \left( 1 - \text{carrier-phonon interaction} \right)^2}$$

(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

\[
\frac{i}{\hbar} \chi(k, \omega) = \frac{\chi}{1 - \chi} = \frac{\chi}{D_1} + \frac{\chi}{D_2}
\]

- the phonon dressed line governed by this equation:

\[
\frac{i}{\hbar} D(k, \omega) = \frac{\chi}{1 - \chi} = \frac{\chi}{D_6} + \frac{\chi}{D_7}
\]

- and the dressed interaction given by:

\[
-\frac{i}{\hbar} g^\text{eff}_q = \frac{\chi}{1 - \chi}
\]

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 $W^\text{ph}(q; t_1 t_2)$:

\[
\chi(q; t_1 t_2) = \pi(q; t_1 t_2) + \int dt_3 V_q \pi(q; t_1 t_3) \chi(q; t_3 t_2)
\]

\[
D(q; t_1 t_2) = D^{(0)}(q; t_1 t_2) + \int dt_3 \int dt_4 g^2_q D^{(0)}(q; t_1 t_3) \chi(q; t_3 t_4) D(q; t_4 t_2)
\]

\[
W^\text{ph}(q; t_1 t_2) = \int dt_3 \int dt_4 g^2_q \epsilon^{-1}(q; t_1 t_3) D(q; t_3 t_4) \epsilon^{-1}(q; t_4 t_2)
\]
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

\[
\frac{dG(11')}{dU(3)} = \frac{i}{\hbar} \left( T \left\{ \frac{dS_{\text{ext}}^{(t_0, t_0)} \hat{\psi}_H(1) \hat{\psi}_H(1')}{} \right\} \right) \frac{\langle S_{H}^{(t_0, t_0)} \rangle}{\langle S_{\text{ext}}^{(t_0, t_0)} \rangle} \left( \frac{dS_{H}^{(t_0, t_0)}}{dU(3)} \right) - \left( \frac{i}{\hbar} \right)^2 \left( T \left\{ \frac{S_{\text{ext}}^{(t_0, t_0)} \hat{\psi}_H(1) \hat{\psi}_H(1')}{} \right\} \right) \frac{\langle S_{\text{ext}}^{(t_0, t_0)} \rangle}{\langle S_{H}^{(t_0, t_0)} \rangle} \frac{\langle S_{\text{ext}}^{(t_0, t_0)} \rangle}{\langle S_{H}^{(t_0, t_0)} \rangle} + G(11') \cdot \left( \frac{i}{\hbar} \right) \left( T \left\{ \frac{S_{\text{ext}}^{(t_0, t_0)} \hat{\psi}_H(3) \hat{\psi}_H(1')}{} \right\} \right) \frac{\langle S_{\text{ext}}^{(t_0, t_0)} \rangle}{\langle S_{H}^{(t_0, t_0)} \rangle} = -G(13^{-1} 1' 3^+ - G(11')G(33^+). \tag{F.1}
\]
Inserting this final result into equation (2.2) yields

\[
\left( i \frac{\text{d}}{\text{d}t_1} + \frac{\hbar^2 \nabla_i^2}{2m} - U(1) \right) G(11') = \delta(11') + i\hbar \int_C \text{d}3 \: V(1-3) \frac{\text{d}G(11')}{\text{d}U(3)} \\
- i\hbar \int_C \text{d}3 \: V(1-3)G(33')G(11') \]

\[
= \delta(11') + \int_C \text{d}2 \Sigma_{\text{tot}}(12)G(21')
\]

(F.2)

where the total self-energy \( \Sigma_{\text{tot}}(12) = \Sigma_{\text{Hartree}}(12) + \Sigma(12) \). First, the Hartree self-energy \( \Sigma_{\text{Hartree}}(12) \) will be considered. If one compares the first and the second line of equation (F.2), one finds that

\[
\Sigma_{\text{Hartree}}(12) = -i\hbar \delta(12) \int_C \text{d}3 \: V(1-3)G(33')
\]

(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

\[
\int_C \text{d}2 \: G^{-1}(12)G(21') = \int_C \text{d}2 \: G(12)G^{-1}(21') = \delta(11')
\]

(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

\[
i\hbar \int_C \text{d}3 \: V(1-3) \frac{\text{d}G(11')}{\text{d}U(3)} = i\hbar \int_C \text{d}3 \int_C \text{d}4 \: V(1-3) \frac{\text{d}G(14)}{\text{d}U(3)} \delta(41') \\
= i\hbar \int_C \text{d}2 \int_C \text{d}3 \int_C \text{d}4 \: V(1-3) \frac{\text{d}G(14)}{\text{d}U(3)} G^{-1}(42)G(21') \\
= \int_C \text{d}2 \int_C \Sigma(12)G(21')
\]

(F.5)

and

\[
\Sigma(12) = i\hbar \int_C \text{d}3 \int_C \text{d}4 \: V(1-3) \frac{\text{d}G(14)}{\text{d}U(3)} G^{-1}(42).
\]

(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 $U_{\text{eff}}(1)$, containing both $U(1)$ and the Hartree self-energy $\Sigma_{\text{Hartree}}(12)$, with

$$U_{\text{eff}}(1) = U(1) - i \int_C d2 V(1 − 2) G(22^+) \cdot (22) \cdot (22) \cdot (22) \cdot (22) \cdot (22) \cdot (22).$$  

One starts from equation (F.6) and repeatedly changes variables:

$$\Sigma(12) = i \int_C d3 \int_C d4 V(1 − 3) \frac{dG(14)}{dU(3)} G^{-1}(42) \cdot (42) \cdot (42) \cdot (42) \cdot (42) \cdot (42) \cdot (42).$$

The transition from the first line to the second was obtained because

$$\frac{d}{dU(3)} \left[ \int_C d2 G(12) G^{-1}(21') \right] = \frac{d(11')}{dU(3)} = 0 = \int_C d2 \frac{dG(12)}{dU(3)} G^{-1}(21') + \int_C d2 G(12) \frac{dG^{-1}(21')}{dU(3)}.$$  

In going from the third to the fourth line, one introduced the screened Coulomb potential

$$W(21) = \int_C d3 V(1 − 3) \frac{dU_{\text{eff}}(2)}{dU(3)},$$

and the vertex function

$$\Gamma(123) = \frac{dG^{-1}(12)}{dU_{\text{eff}}(3)}.$$
Recalling the definition of $U_{\text{eff}}(1)$ from equation (F.7) and inserting it into (F.10) yields

$$\frac{dU_{\text{eff}}(1)}{dU(2)} = \delta(12) - i\hbar \int_C d^3V(1-3) \frac{dG(33^+)}{dU(2)} = \delta(12) - i\hbar \int_C d^3 \int_C d^4V(1-3) \frac{dG(33^+)}{dU_{\text{eff}}(4)} \frac{dU_{\text{eff}}(4)}{dU(2)} \quad (F.12)$$

and

$$W(21) = V(1-2) - i\hbar \int_C d^3 \int_C d^4 \int_C d^5V(1-3)V(2-4) \frac{dG(44^+)}{dU_{\text{eff}}(5)} \frac{dU_{\text{eff}}(5)}{dU(3)}$$

$$= V(1-2) - i\hbar \int_C d^3 \int_C d^4 \int_C d^5 V(2-4) \frac{dG(44^+)}{dU_{\text{eff}}(5)} W(51)$$

$$= V(1-2) + \int_C d^4 \int_C d^5 V(2-4) \pi(45) W(51), \quad (F.13)$$

where the polarization function is defined in the following way

$$\pi(12) = -i\hbar \frac{dG(11^+)}{dU_{\text{eff}}(2)}$$

$$= -i\hbar \int_C d^3 \int_C d^4 \frac{dG(13)}{dU_{\text{eff}}(2)} G^{-1}(34) G(41^+)$$

$$= i\hbar \int_C d^3 \int_C d^4 G(13) \frac{dG^{-1}(34)}{dU_{\text{eff}}(2)} G(41^+)$$

$$= i\hbar \int_C d^3 \int_C d^4 G(13) \Gamma(342) G(41^+). \quad (F.14)$$

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)

$$\left(i\hbar \frac{dt_1}{dt} + \frac{\hbar^2 \nabla^2}{2m} - U_{\text{eff}}(1) \right) G(12) = \int_C d^3 \left[ G_{\text{eff}}^{(0)}(13) \right]^{-1} G(32)$$

$$= \delta(12) + \int_C d^3 \Sigma(13) G(32) \quad (F.15)$$

with

$$\left[ G_{\text{eff}}^{(0)}(12) \right]^{-1} = \left(i\hbar \frac{dt_1}{dt} + \frac{\hbar^2 \nabla^2}{2m} - U_{\text{eff}}(1) \right) \delta(12). \quad (F.16)$$

Multiplying and integrating each line of equation (F.15) by $\int_C d^2 G^{-1}(21')$, one finds that

$$\left[ G_{\text{eff}}^{(0)}(11') \right]^{-1} = G^{-1}(11') + \Sigma(11') \quad (F.17)$$
or

\[ G^{-1}(11') = \left[ G_{eff}^{(0)}(11') \right]^{-1} - \Sigma(11'). \]  \hspace{1cm} (F.18)

The vertex function \( \Gamma \) is now defined by

\[
\Gamma(123) = \frac{dG^{-1}(12)}{dU_{eff}(3)}
- \frac{d\Sigma(12)}{dU_{eff}(3)}
= -\delta(12')\delta(13) - \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG^{(45)}} \frac{dG^{(45)}}{dU_{eff}(3)} \int_C d6 \int_C d7 \frac{dG^{(45)}}{dU_{eff}(3)} G^{-1}(67)G(75)
\]

\[
= -\delta(12')\delta(13)
- \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG^{(45)}} \int_C d6 \int_C d7 \frac{dG^{(45)}}{dU_{eff}(3)} G^{-1}(67)G(75)
\]

\[
= -\delta(12')\delta(13)
+ \int_C d4 \int_C d5 \frac{d\Sigma(12)}{dG^{(45)}} \int_C d6 \int_C d7 \frac{dG^{(45)}}{dU_{eff}(3)} G(46)\Gamma(673)G(75). \]  \hspace{1cm} (F.19)

This is the starting point of the perturbation theory. The equation for the vertex function \( \Gamma \) is reiterated and each time inserted in the equations for the polarization function \( \pi \), the screened Coulomb potential \( W \) and the self-energy \( \Sigma \), which in turn contributes to the next iteration of \( \Gamma \):

\[
\Gamma = \Gamma^{(0)} + \Gamma^{(1)}(\Sigma^{(0)}, \Gamma^{(0)}) + \Gamma^{(2)}(\Sigma^{(1)}, \Gamma^{(1)}, \Sigma^{(0)}, \Gamma^{(0)}) + \cdots
\]

\[
\pi = \pi^{(0)}(\Gamma^{(0)}) + \pi^{(1)}(\Gamma^{(1)}) + \pi^{(2)}(\Gamma^{(2)}) + \cdots
\]

\[
W = W^{(0)}(\pi^{(0)}) + W^{(1)}(\pi^{(1)}) + W^{(2)}(\pi^{(2)}) + \cdots
\]

\[
\Sigma = \Sigma^{(00)}(W^{(0)}, \Gamma^{(0)}) + \Sigma^{(10)}(W^{(1)}, \Gamma^{(0)}) + \Sigma^{(01)}(W^{(0)}, \Gamma^{(1)}) + \cdots \]  \hspace{1cm} (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 \( \pi \) is replaced by

\[
\pi(12) = \pi^{(0)}(12)
= i\hbar \int_C d3 \int_C d4 G(13)\Gamma^{(0)}(342)G(41^+)
= -i\hbar G(12)G(21^+) \]  \hspace{1cm} (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

\[
\Sigma(12) = \Sigma^{(0)}(12) = -i\hbar \int d4 \int d5 W^{(0)}(51)G(14)\Gamma^{(0)}(425) = i\hbar \int d4 \int d5 W_{RPA}(51)G(14)\delta(42)\delta(45)
\]

\[
= i\hbar W_{RPA}(21)G(12).
\] (F.22)

For the later treatment of the time dependence of the self-energy \( \Sigma \), it is convenient to separate it into two parts resulting from equation (F.13) for the screened potential

\[
\Sigma(12) = i\hbar W_{RPA}(21)G(12) = i\hbar V(1 - 2)G(12) + i\hbar \int d4 \int d5 V(2 - 4)\pi(45)W_{RPA}(51)G(12).
\] (F.23)

\section*{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

\[
\Sigma_{\text{Fock}}(12) = i\hbar V(1 - 2)G(12)
\] (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]

\[
\Sigma^{\text{tot}}(12) = \Sigma^{\delta}(12) + \Sigma(12)
\] (F.25)

with

\[
\Sigma^{\delta} = \Sigma_{\text{Hartree}} + \Sigma_{\text{Fock}} = i\hbar V(1 - 2)G(12) - i\hbar \delta(12) \int d3 V(1 - 3)G(33^+).
\] (F.26)

\section*{F.1.2 Direct Collision Self-Energy}

The second part of equation (F.23) is the direct collision self-energy given by

\[
\Sigma_{\text{dc}}(12) = i\hbar \int d3 \int d4 V(2 - 3)\pi(34)W(41)G(12).
\] (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 $\Sigma^{01}$ where the vertex function $\Gamma^{(1)}(123)$ occurs.

$$
\Gamma^{(1)}(123) = \int d4 \int d5 \int d6 \int d7 d\Sigma^{(0)(12)} dG(46) G(75) 
$$

$$
= -\int d4 \int d5 \frac{d\Sigma^{(0)(12)}}{dG(45)} G(43) G(35) \quad (F.28)
$$

where

$$
\frac{d\Sigma^{(0)(12)}}{dG(45)} = i\hbar W(21) \frac{dG(12)}{dG(45)} 
$$

$$
= i\hbar W(21) \delta(14) \delta(25). \quad (F.29)
$$

Therefore $\Gamma^{(1)}$ becomes

$$
\Gamma^{(1)}(123) = -i\hbar W(21) G(13) G(32). \quad (F.30)
$$

This gives for the self-energy $\Sigma_{ex}(12) = \Sigma^{(01)(12)}$, which describes the exchange collision effects:

$$
\Sigma_{ex}(12) = -i\hbar \int d3 \int d4 W(31) G(14) \Gamma^{(1)}(423) 
$$

$$
= - (\hbar)^2 \int d3 \int d4 W(31) G(14) G(43) G(32) W(42) \quad (F.31)
$$

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

$$
V^{c-n} = \int d2 \ V(1-2) \rho^n(2), \quad (F.32)
$$

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

$$
H^{c-n} = \int d1 \int d2 \ V(1-2) \hat{\psi}^\dagger(1) \hat{\psi}(1) \rho^n(2) 
$$

$$
= \int d1 \int d2 \ V(1-2) \rho^{el}(1) \rho^n(2). \quad (F.33)
$$
Then the total Hamiltonian \( H(t) \) contains the unperturbed part \( H^0 \), the carrier-carrier interaction \( V \), the carrier-nuclei interaction \( H^{c-n} \) and an external perturbation \( H^{\text{ext}}(t) \) acting both on the carriers and the nuclei

\[
H^{\text{ext}}(t) = \int dx \ U(x,t) \left( \rho^c(x,t) + \rho^n(x,t) \right). \tag{F.34}
\]

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

\[
\left( i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla^2}{2m} - U(1) - \int_C d^3 V(1 - 3) \langle \rho^n(3) \rangle \right) G(11') =
\]

\[
\delta(11') - i\hbar \int_C d^3 V(1 - 3) G(2) (13^+23^+). \tag{F.35}
\]

This is done with

\[
\frac{i\hbar}{dt} \left\{ \frac{d}{dt} \left( S_{\text{H}}^{\text{ext}}(t_0,t_0) \hat{\psi}_H(x,t) \right) \right\} =
\]

\[
T \left\{ \frac{i\hbar}{dt} \left( S_{\text{H}}^{\text{ext}}(t_0,t) \hat{\psi}_H(x,t) S_{\text{H}}^{\text{ext}}(t,t_0) \right) \right\}
\]

\[
= T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) \frac{i\hbar}{dt} \hat{\psi}_H(x,t) \right\}
\]

\[
+ i\hbar T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) \int dx_2 U(x_2,t) \left[ \hat{\psi}_H(1), \rho^c(x_2) + \rho^n(x_2) \right] \right\}
\]

\[
= T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) \frac{i\hbar}{dt} \hat{\psi}_H(x,t) \right\} + i\hbar T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) U(1) \hat{\psi}_H(1) \right\}
\]

and

\[
\frac{i\hbar}{dt} \hat{\psi}_H(x,t) = \left[ \hat{\psi}_H(x,t), H_H(t) \right]
\]

\[
= -\frac{\hbar^2 \nabla^2}{2m} \hat{\psi}_H(x,t) + \int dy \ V(x-y) \hat{\psi}_H(y,t) \hat{\psi}_H(y,t) \hat{\psi}_H(x,t)
\]

\[
+ \int dy \ V(x-y) \rho^n(y,t) \hat{\psi}_H(x,t).
\]

Furthermore, modifying equation (F.1) to take into account the carrier-phonon interaction yields

\[
\frac{dG(11')}{dU(3)} = -\left( \frac{i}{\hbar} \right)^2 \frac{T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) \hat{\psi}_H(1) \left( \hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) + \rho^n(3) \right) \hat{\psi}_H^\dagger(1') \right\}}{\langle S_{\text{H}}^{\text{ext}}(t_0,t_0) \rangle}
\]

\[
+ G(11') \cdot \left( \frac{i}{\hbar} \right) \frac{T \left\{ S_{\text{H}}^{\text{ext}}(t_0,t_0) \left( \hat{\psi}_H(3) \hat{\psi}_H^\dagger(3) + \rho^n(3) \right) \right\}}{\langle S_{\text{H}}^{\text{ext}}(t_0,t_0) \rangle}
\]

\[
= -G(13^+13^+13^+) - G(11') A(3) + G(11') \left( G(33^+) + A(3) \right)
\]

\[
= -G(13^+13^+13^+) + G(11') G(33^+), \tag{F.36}
\]
where
\[
A(3) = -\frac{i}{\hbar} \langle T \{ S^{\text{eff}}_{\text{H}}(t_0, t_0) \rho^n(3) \} \rangle.
\]

Using equation (F.36) and the equality \( \langle \rho^{el}(1) \rangle = -\frac{i}{\hbar} G(11^+) \) allows to rewrite equation (F.35) as
\[
(i/\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U(1) - \int_C d^3 V (1 - 3) \left( \langle \rho^{el}(3) \rangle + \langle \rho^n(3) \rangle \right) ) G(11') =
\]
\[
\delta(11') + ih \int_C d^3 V (1 - 3) \frac{dG(11')}{dU(3)}.
\]

Therefore, with the same procedure as at the beginning of this Appendix, one obtains for the effective external potential
\[
U_{eff}(1) = U(1) - ih \int_C d^2 V (1 - 2) G(22^+) + \int_C d^2 V (1 - 2) \langle \rho^n(2) \rangle
\]
\[
= U(1) + \int_C d^2 V (1 - 2) \left( \langle \rho^{el}(2) \rangle + \langle \rho^n(2) \rangle \right)
\]
\[
\text{(F.37)}
\]
which implies
\[
\left( i\hbar \frac{d}{dt_1} + \frac{\hbar^2 \nabla_1^2}{2m} - U_{eff}(1) \right) G(11') = \delta(11') + ih \int_C d^3 V (1 - 3) \frac{dG(11')}{dU(3)}.
\]
\[
\text{(F.38)}
\]

In order to compute the carrier-phonon interaction, one has to introduce a source term in the external Hamiltonian \( H^{\text{ext}}(t) \) from equation (F.34) [13]
\[
H^{\text{ext}}(t) = \int dx \left[ U(x, t) \left( \rho^{el}(x, t) + \rho^n(x, t) \right) + J(x, t) \rho^n(x, t) \right]. \quad \text{(F.39)}
\]

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
\[
\frac{dU_{eff}(1)}{dU(2)} = \delta(12) + \int_C d^3 V (1 - 3) \left( \frac{d\langle \rho^{el}(3) \rangle}{dU(2)} + \frac{d\langle \rho^n(3) \rangle}{dU(2)} \right)
\]
\[
= \delta(12) - ih \int_C d^3 \int_C d^4 V (1 - 3) \frac{dG(33^+)}{dU_{eff}(4)} \frac{dU_{eff}(4)}{dU(2)}
\]
\[
+ \int_C d^3 V (1 - 3) \frac{d\langle \rho^n(3) \rangle}{dU(2)}. \quad \text{(F.40)}
\]

One can rewrite this equation
\[
\int_C d^4 K(14) \frac{dU_{eff}(4)}{dU(2)} = \delta(12) + \int_C d^3 V (1 - 3) \frac{d\langle \rho^n(3) \rangle}{dU(2)} \quad \text{(F.41)}
\]
with
\[ K(12) = \delta(12) + i\hbar \int_C d3 V(1-3) \frac{dG(33^+)}{dU_{eff}(2)} \] (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)
\[ \epsilon^{-1}(12) = \frac{dU_{el}^{el}}{dU(2)} = \delta(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}^0(4)} \epsilon^{-1}(42), \] (F.43)

where \( U_{eff}^{el} \) contains only the influence of carrier-carrier scattering. Assuming that for weak carrier-phonon interaction \( U_{eff} \approx U_{eff}^{el} \), one finds
\[ K(12) = \epsilon(12) \] (F.44)
because of equation (F.43) and
\[
\int_C d4 K(14) \epsilon^{-1}(42) = \epsilon^{-1}(12) - i\hbar \int_C d3 \int_C d4 V(1-3) \frac{dG(33^+)}{dU_{eff}^0(4)} \epsilon^{-1}(42) \\
\approx \delta(12). \] (F.45)

The consequence for equation (F.41) is
\[
\frac{dU_{eff}(4)}{dU(2)} = \epsilon^{-1}(12) + \int_C d3 \int_C d4 \epsilon^{-1}(13) V(3-4) \frac{d\langle \rho^n(4) \rangle}{dU(2)} \\
= \epsilon^{-1}(12) + \int_C d3 W(13) \frac{d\langle \rho^n(3) \rangle}{dU(2)}. \] (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
\[
\langle \rho^n(1) \rangle = \frac{T\{S\rho^n(1)\}}{\langle S \rangle}. \] (F.47)

This enables to calculate the reaction of the nuclei under the action of the external potential \( U(x,t) \)
\[
\frac{d\langle \rho^n(1) \rangle}{dU(2)} = -\frac{i}{\hbar} \langle T\{S\rho^n(1)\}\rangle \frac{T\{S\rho^n(1)\}}{\langle S \rangle} \] (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

$$
\frac{d\langle \rho^n(1) \rangle}{dJ(2)} = -\frac{i}{\hbar} \frac{\langle T \{ \Delta \rho^n(2) \Delta \rho^n(1) \} \rangle}{\langle S \rangle} = \mathcal{D}(12) \tag{F.49}
$$

and

$$
\frac{d\langle \rho^el(1) \rangle}{dJ(2)} = -\frac{i}{\hbar} \frac{\langle T \{ \Delta \rho^n(2) \Delta \rho^el(1) \} \rangle}{\langle S \rangle}. \tag{F.50}
$$

Going back to equation (F.48), one finds

$$
\frac{d\langle \rho^n(1) \rangle}{dU(2)} = \frac{d\langle \rho^n(2) \rangle}{dJ(1)} + \frac{d\langle \rho^el(2) \rangle}{dJ(1)} = \mathcal{D}(12) + \int_C d^3 \frac{d\langle \rho^el(2) \rangle}{dU_{eff}(3)} \frac{dU_{eff}(3)}{dJ(1)} \tag{F.51}
$$

or

$$
\int_C d^4 \frac{d\langle \rho^n(1) \rangle}{dU(4)} L(42) = \mathcal{D}(12) \tag{F.52}
$$

with

$$
L(12) = \delta(12) - \int_C d^3 V(1 - 3) \frac{d\langle \rho^el(2) \rangle}{dU_{eff}(3)} \tag{F.53}
$$

Comparing equations (F.42) and (F.53) shows that they are similar, except for the arguments 2 and 3 in $\pi(23) = \frac{dG(22^+)}{dU_{eff}(3)}$, 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,

$$
\frac{d\langle \rho^n(1) \rangle}{dU(2)} = \int_C d^3 \mathcal{D}(13) \epsilon^{-1}(32) \tag{F.54}
$$

and the insertion of this result into equation (F.46) gives

$$
\frac{dU_{eff}(1)}{dU(2)} = \epsilon^{-1}(12) + \int_C d^3 \int_C d^4 W(13) \mathcal{D}(34) \epsilon^{-1}(42) = \epsilon_{eff}^{-1}(12). \tag{F.55}
$$
With this equation, it is possible to compute the total screened potential \( W_{\text{eff}}(12) \) 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

\[
W_{\text{eff}}(21) = \int_C d^3V (1 - 3) e^{-1}_{eff}(23) = W_{el}(21) + \int_C d^3 \int_C d^4 W_{el}(23) D(34) W_{el}(41). \tag{F.56}
\]

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

\[
H^{FR} = \int dr \, \hat{\psi}^\dagger(r) \sum_q \frac{e^{iqr}}{|q|} \left( C a_q + C^* a^-_{-q} \right) \hat{\psi}(r) \tag{F.57}
\]

where \( a_q \) and \( a^\dagger_{-q} \) are the annihilation and creation phonon operators, respectively and

\[
C = \sqrt{\frac{e^2}{V^2} \frac{\hbar \omega_{LO}}{2} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)}. \tag{F.58}
\]

\( C \) is the Fröhlich constant. Therefore, comparing this Hamiltonian with the Hamiltonian of equation (F.33), one finds

\[
H^{FR}(1) = \int d^3V (1 - 3) \rho^n(3) \tag{F.59}
\]

and

\[
\rho^n(1) = \int d^3V^{-1}(1 - 3) H^{FR}(3) \tag{F.60}
\]

This results is inserted into equation (F.49) and after some algebra, one finds for \( D(12) \)

\[
D(12) = \frac{i}{\hbar} \frac{\langle T\{S \Delta \rho^n(2) \Delta \rho^n(1)\}\rangle}{\langle S \rangle} = \int d^3 \int d^4 \sum_{q_1 q_2} \frac{|C|^2}{|q_1||q_2|} e^{iq_1 r_1} e^{iq_2 r_4} V^{-1}(1 - 3) V^{-1}(2 - 4) D(q_1 q_2; t_3 t_4) \tag{F.61}
\]
where $D(q_1 q_2; t_3 t_4)$ is the phonon Green’s function and is defined as

$$D(q_1 q_2; t_3 t_4) = -i \frac{\langle T \{ S A_\uparrow(q_1, t_1) A(q_2, t_2) \} \rangle}{\langle S \rangle}$$

with $A(q, t) = a_\uparrow(t) + a_{-q}(t)$. 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

$$a_q(t) = e^{iH_0 t/\hbar} a_q e^{-iH_0 t/\hbar}$$

and therefore [5]

$$D^>_0(q, t) = -\frac{i}{\hbar} \left[ (N_q + 1) e^{-i\omega_q t} + N_q e^{i\omega_q t} \right]$$

$$D^<_0(q, t) = -\frac{i}{\hbar} \left[ (N_q + 1) e^{i\omega_q t} + N_q e^{-i\omega_q t} \right]$$

$$D^R_0(q, t) = -\frac{2}{\hbar} \theta(t) \sin(\omega_q t)$$

$$D^A_0(q, t) = \frac{2}{\hbar} \theta(-t) \sin(\omega_q t)$$

... (F.64)

By inserting equation (F.61) into (F.56), an expression is found for the effective potential where carrier-phonon interaction is present

$$W_{ph}(21) = \int_C d3 \int_C d4 \int_C d5 \int_C d6 \sum_{q_1 q_2} \left| C_{q_1 q_2} \right|^2 e^{i q_1 r_5} e^{i q_2 r_6} W_{el}(23) V^{-1}(3 - 5)$$

$$V^{-1}(4 - 6) W_{el}(41) D(q_1 q_2; t_5 t_6).$$

(F.65)

According to equation (F.22), the self-energy accounting for carrier-phonon interaction is derived

$$\Sigma^{ph}(12) = i\hbar W_{ph}(21) G(12).$$

(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

$$\int_C d3 \ V(1 - 3) V(3 - 2) = \delta(12),$$

(F.67)

and the carrier-phonon self-energy is

$$\Sigma^{ph}(12) = i\hbar \sum_{q_1 q_2} \left| C_{q_1 q_2} \right|^2 e^{i q_1 r_1} e^{i q_2 r_2} D(q_1 q_2; t_1 t_2) G(12).$$

(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

$$H_{ph} = \int d^3x \hat{\psi}^\dagger(x) \sum_q e^{iqx} M(q) \hat{\psi}(x)$$

is added to the total Hamiltonian of (2.1). This gives

$$i\hbar \left( \frac{d}{dt_1} + \frac{d}{dt_2} \right) G(12) + \frac{\hbar^2}{2m} \left[ (\nabla_{x_1} + \nabla_{x_2})(\nabla_{x_1} - \nabla_{x_2}) \right] G(12) =$$

$$(U(1) - U(2)) G(12) - i\hbar \int_C d3 \ (V(1 - 3) - V(2 - 3)) G^{(2)}(13-23^+)$$

$$- \frac{i}{\hbar} \sum_q C_q (e^{iqx_1} - e^{iqx_2}) \langle T \left\{ \hat{\psi}_H(1) \left( a_q - a_{-q}^\dagger \right) \hat{\psi}_H(2) \right\} \rangle =$$

$$(U(1) - U(2)) G(12) + \int_C d3 \ \Sigma^{tot(13)} G(32) - G(13) \Sigma^{tot(32)} \right). \quad (G.1)$$

The last equality results from equations (2.5) and (2.6). By taking the limit $x_2 \to x_1$ and $t_2 \to t_1^+$, one obtains

$$i\hbar \frac{d}{dt_1} G^< (x_1 t_1; x_1 t_1) + \nabla_{x_1} \left( \frac{\hbar^2}{2m} \lim_{x_2 \to x_1} (\nabla_{x_1} - \nabla_{x_2}) G^< (x_1 t_1; x_2 t_1) \right) = 0. \quad (G.2)$$

Recalling the definition of the carrier density from equation (1.32) yields

$$- \frac{d}{dt_1} n(x_1, t_1) + \nabla_{x_1} \left( \frac{\hbar^2}{2m} \lim_{x_2 \to x_1} (\nabla_{x_1} - \nabla_{x_2}) G^< (x_1 t_1; x_2 t_1) \right) = 0. \quad (G.3)$$

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

\[
J(x_1, t_1) = \frac{\hbar^2}{2m} \lim_{x_2 \to x_1} (\nabla x_2 - \nabla x_1) G^<(x_1 t_1; x_2 t_1). \tag{G.5}
\]

The equivalence of the second and the third equalities of equation (G.1) implies in the limit \( x_2 \to x_1 \) and \( t_2 \to t_1 \) that

\[
\int_C d\mathbf{q} \left( \Sigma_{tot}(x_1 t_1; x_3 t_3)G(x_3 t_3; x_1 t_1) - G(x_1 t_1; x_3 t_3)\Sigma_{tot}(x_3 t_3; x_1 t_1) \right) = 0. \tag{G.6}
\]

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)

\[
\sum_{k,l} \int \frac{dE}{2\pi} \left( \Sigma_{nl}^R(k; E)G_{ln}^<(k; E) + \Sigma_{nl}^< (k; E)G_{ln}^A(k; E) - \right.
\]

\[
G_{nl}^R(k; E)\Sigma_{ln}^< (k; E) - G_{nl}^<(k; E)\Sigma_{ln}^A (k; E) \bigg) = 0. \tag{G.7}
\]

The self-energies \( \Sigma_{nl}^R(k; E) \), \( \Sigma_{nl}^< (k; E) \), and \( \Sigma_{ln}^A (k; E) \) are given in equation (2.65).

Due to the pseudo-Wannier functions basis, the matrix element \( M_{n_1 n_2}(q) \) can be written as

\[
M_{n_1 n_2}(q) = \left| \frac{C}{q} e^{i q s (z_{n_1} - z_{n_2})} \right|. \tag{G.8}
\]

Taking a look at the form of equation (G.7) and of the self-energies, one sees that the term \( G_{nl}^R(k; E)\Sigma_{ln}^< (k; E) \) can compensate one part of \( \Sigma_{nl}^R(k; E)G_{ln}^<(k; E) \) for each different index \( l \)

\[
\sum_{k, q} \int \frac{dE}{2\pi} \left[ \frac{C^2}{q^2} \left( e^{i q l (z_{n_1} - z_l)} \left( (N_q + 1)G_{nl}^<(k - q_l; E - \hbar \omega_q) + N_q G_{nl}^<(k - q_l; E + \hbar \omega_q) \right) G_{ln}^<(k; E) \right.ight.
\]

\[
- G_{nl}^<(k; E)e^{i q l (z_l - z_{n_1})} \left( N_q G_{ln}^<(k - q_l; E - \hbar \omega_q) + (N_q + 1)G_{ln}^<(k - q_l; E + \hbar \omega_q) \right) \bigg].
\]
G.2 Example

One immediately sees that this term is equal to zero if one makes some variable transformations: first, in the second line $q$ is replaced by $-q'$ (sum over $q'$ instead of $q$) and thus $k + q'_||$ by $k'$ (sum over $k'$, $G_{nl}^<(k; E) \rightarrow G_{nl}^<(k' - q'_||; E)$). Then, still for the second line, the terms depending on $N_q$ and $N_q + 1$ must be treated separately:

- $E - \hbar \omega_q$ becomes $E'$, the integral over $E$ an integral over $E'$, and the Green’s function $G_{nl}^<(k' - q'_||; E) \rightarrow G_{nl}^<(k' - q'_||; E' + \hbar \omega_q)$. This term is canceled by the second one of the first line.

- $E + \hbar \omega_q$ is replaced by $E'$, the integral over $E$ by an integral over $E'$, and finally $G_{nl}^<(k' - q'_||; E) \rightarrow G_{nl}^<(k' - q'_||; E' - \hbar \omega_q)$. 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

\[ G(11') = \frac{i}{\hbar} \frac{tr(T\{\hat{\psi}_H(x,t)\hat{\psi}^\dagger_H(x',t')\})}{tr(\rho(t_0))}. \] (H.1)

\( \rho(t_0) \) describes the initial state of the system and contains one- and two-particle operators

\[ \rho(t_0) = e^{-B} = e^{-(B^{(0)} + B^{(1)})}, \] (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 \( \hat{\psi}^\dagger_H(x',t') \) 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

\[ H = \int dx \hat{\psi}^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(x) + \frac{1}{2} \int dx \int dy \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)V(x-y)\hat{\psi}(y)\hat{\psi}(x). \]

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

$$
\rho(t_0) = e^{-B} = e^{B_{x_0}}e^{-B^{(0)}_{x_0}}e^{-B^{(0)}_{x_0+1}}e^{-B(x_0+1)}
$$

(H.3)

with $-1 \leq x_0 \leq 0$. One defines two new quantities, $U_1(\tau) = e^{B^{(0)}_x}e^{-B_\tau}$ with $\tau > 0$ and its parent $U_2(\tau) = e^{B^{(0)}_x}e^{-B^{(0)}_\tau}$ where $\tau < 0$. With some algebra similar to Appendix A, one finds for $U_1(\tau)$

$$
U_1(\tau)\big|_{\tau > 0} = T^c \left\{ \exp \left( -\int_0^\tau d\tau' B^{(1)}_I(\tau') \right) \right\}.
$$

(H.4)

For $U_2(\tau)$, the procedure is the same as in Appendix B, except that $T^s$ is replaced by $T^c$ because $\tau$ is smaller than 0.

$$
U_2(\tau)\big|_{\tau < 0} = T^c \left\{ \exp \left( \int_0^\tau d\tau' B^{(1)}_I(\tau') \right) \right\}
\quad = T^c \left\{ \exp \left( -\int_\tau^0 d\tau' B^{(1)}_I(\tau') \right) \right\}.
$$

(H.5)

The index $I$ in $B^{(1)}_I(\tau')$ represents a time evolution in the interaction picture

$$
B^{(1)}_I(\tau') = e^{\tau B^{(0)}_I}B^{(1)}_I e^{-\tau B^{(0)}_I}.
$$

(H.6)

Obviously, the definitions for $U_1$ and $U_2$ are identical and one can introduce an evolution operator $S^B_I(\tau_1, \tau_2)$ ($I$ because interaction picture and $B$ because relative to the $B$ operator) with

$$
S^B_I(\tau_1, \tau_2)|_{\tau_1 > \tau_2} = T^c \left\{ \exp \left( -\int_{\tau_2}^{\tau_1} d\tau' B^{(1)}_I(\tau') \right) \right\}
$$

(H.7)

and relate it to $U_1$ and $U_2$

$$
U_1(\tau)|_{\tau > 0} = S^B_I(\tau, 0), \quad U_2(\tau)|_{\tau < 0} = S^B_I(0, \tau).
$$

(H.8)

These results are inserted in the definition of the Green’s function

$$
G(11') = \frac{i}{\hbar} \frac{\text{tr} \left\{ S^B_I(0, x_0)e^{-B^{(0)}_I}S^B_I(x_0 + 1, 0)T \left\{ \hat{\psi}_H(x, t)\hat{\psi}^+_H(x', t') \right\} \right\}}{\text{tr} \left\{ S^B_I(0, x_0)e^{-B^{(0)}_I}S^B_I(x_0 + 1) \right\}}
\quad = -\frac{i}{\hbar} \frac{\langle S^B_I(x_0 + 1, 0)T \left\{ \hat{\psi}_H(x, t)\hat{\psi}^+_H(x', t') \right\} S^B_I(0, x_0) \rangle_0}{\langle S^B_I(x_0 + 1, x_0) \rangle_0}.
$$

(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

\[
\hat{\psi}_H(x,t) = S^I_H(t_0,t) \hat{\psi}_I(x,t) S^I_H(t,t_0)
\]

\[
\hat{\psi}^\dagger_H(x',t') = S^I_H(t_0,t') \hat{\psi}^\dagger_I(x',t') S^I_H(t',t_0)
\]

where one has for the time evolution \( S^I_H \) in the interaction picture and relative to \( H \)

\[
S^I_H(t,t') = T^v \left\{ \exp \left( -\frac{i}{\hbar} \int_{t'}^t dt_1 H^{(1)}_I(t_1) \right) \right\}, \quad \text{with} \quad v = \left\{ \begin{array}{ll} c, & t > t' \\ a, & t' > t \end{array} \right.
\]

and

\[
H^{(1)}_I(t_1) = e^{iH^{(0)}/\hbar} H^{(1)} e^{-iH^{(0)}/\hbar}
\]

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

\[
G(11') = -\frac{i}{\hbar} \frac{\langle S^B_I(x_0 + 1,0) T_C \left\{ \exp \left( -\frac{i}{\hbar} \int_C dt_1 H_I^{(1)}(t_1) \right) \hat{\psi}_I(x,t) \hat{\psi}^\dagger_I(x',t') \right\} S^B_I(0,x_0) \rangle_0}{\langle S^B_I(x_0 + 1,0) \rangle_0},
\]

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 \( C \), 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 real part of the time and \( \tau \) the imaginary one. \( \xi \) goes along the contour \( C \), Figure H.1. The new time-ordering operator \( T_C \) orders the elements of the Green’s function along \( C \). Hence a point on \( C = C^+ + C^- \) is always “earlier” than a point

![Figure H.1: Contour C for the evaluation of the Green’s function with initial correlations. This is the special case, where x0 is equal to 0](image-url)
on $C_\tau$.
Furthermore, one defines an interaction picture with respect to
\begin{equation}
H^{(1)}_I(\xi) = \begin{cases} H^{(1)}_I(t), & \xi \text{ on } C \\ -i\hbar B^{(1)}_I(\tau), & \xi \text{ on } C_\tau \end{cases}
\end{equation}
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
\begin{equation}
G(11') = \frac{-i}{\hbar} \frac{\langle \mathcal{T}_C \{ \exp \left( -\frac{i}{\hbar} \int_C d\xi H^{(1)}_I(\xi) \right) \hat{\psi}_I(x,t) \hat{\psi}^\dagger_I(x',t') \} \rangle_0}{\langle \mathcal{T}_C \{ \exp \left( -\frac{i}{\hbar} \int_C d\xi H^{(1)}_I(\xi) \right) \rangle_0}.
\end{equation}
The contour $C_\tau$ of the denominator was elongated with $C$ to form $C$. 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 $H^{(1)}_I$ is defined on the contour $C$. Therefore, one has to continue $G(11')$ to $C$ and one obtains the $C$-contour-ordered mixed Green’s function $\mathcal{G}(11')$, which means that the time argument of $G$ are on the contour $C$.
\begin{equation}
\mathcal{G}(11') = -\frac{i}{\hbar} \frac{\langle \mathcal{T}_C \{ \exp \left( -\frac{i}{\hbar} \int_C d\xi H^{(1)}_I(\xi) \right) \hat{\psi}_I(1) \hat{\psi}^\dagger_I(1') \} \rangle_0}{\langle \mathcal{T}_C \{ \exp \left( -\frac{i}{\hbar} \int_C d\xi H^{(1)}_I(\xi) \right) \rangle_0}.
\end{equation}
Because Wick’s theorem holds exactly for equation (H.14), the equations of motion for $G(11')$ 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 $\mathcal{G}(11')$, one starts with its definition in the Heisenberg picture, without the expansion for the initial density matrix
\begin{equation}
\mathcal{G}(11') = -\frac{i}{\hbar} \langle \mathcal{T}_C \{ \hat{\psi}^\dagger_H(1) \hat{\psi}^\dagger_H(1') \} \rangle.
\end{equation}
The equation of motion for $\mathcal{G}(11')$ follows directly the equation of motion for the field operators $\hat{\psi}^\dagger_H(1)$ and $\hat{\psi}^\dagger_H(1')$ in the Heisenberg picture on the extended contour.
For an operator \( O_H^B(\tau) = e^{iB}Oe^{-iB} \) in the Heisenberg picture relative to the imaginary time \( \tau \), and the operator \( B \), one has
\[
\frac{i\hbar}{dt} O_H^B(\tau) = [O_H^B(\tau), -i\hbar B_H^B(\tau)]
\]  
(H.16)
and for an operator \( O_H^H(t) = e^{itH/(\hbar)}Oe^{-itH/(\hbar)} \) also in the Heisenberg picture, but for real time \( t \) and with respect to the operator \( H \)
\[
\frac{i\hbar}{dt} O_H^H(t) = [O_H^H(t), H_H^H(t)].
\]  
(H.17)
As in the last section, one defines a common Heisenberg picture with respect to
\[
Q_H(\xi) = \begin{pmatrix} O_H^H(t), & \xi \text{ on } C \\ -i\hbar O_H^B(\tau), & \xi \text{ on } C_\tau \end{pmatrix} \quad \quad \quad H_H(\xi) = \begin{pmatrix} H_H^H(t), & \xi \text{ on } C \\ -i\hbar B_H^B(\tau), & \xi \text{ on } C_\tau \end{pmatrix}
\]
and a common equation of motion
\[
\frac{i\hbar}{d\xi} Q_H(\xi) = [Q_H(\xi), H_H(\xi)].
\]  
(H.18)
Furthermore, \( H_H(\xi) \) is defined as
\[
H_H(\xi) = \int dx \psi_H(x,\xi) \hat{h}(x,\xi) \psi_H(x,\xi) + \frac{1}{2} \int dx \int dy \psi_H(x,\xi) \psi_H^\dagger(y,\xi) V(x,\xi;y,\xi) \psi_H(y,\xi) \psi_H(x,\xi).
\]
with
\[
\hat{h}(x,\xi) = \begin{pmatrix} -\hbar^2 \nabla_x^2/2\hbar, & \xi \text{ on } C \\ -i\hbar \lambda^{(1)}(x), & \xi \text{ on } C_\tau \end{pmatrix} \quad V(x,\xi;y,\xi) = \begin{pmatrix} V(x-y), & \xi \text{ on } C \\ -i\hbar \lambda^{(2)}(x,y), & \xi \text{ on } C_\tau. \end{pmatrix}
\]
To find the paired equations of motion for the mixed Green’s function \( G(11') \), one has to solved both of the following equations
\[
\frac{i\hbar}{d\xi} \hat{\psi}_H(1) = \left[ \hat{\psi}_H(1), H_H(\xi) \right] \quad \frac{i\hbar}{d\xi} \hat{\psi}_H^\dagger(1') = \left[ \hat{\psi}_H^\dagger(1'), H_H(\xi') \right],
\]
where one will concentrate on the first equation
\[
\frac{i\hbar}{d\xi} \hat{\psi}_H(x,\xi) = \hat{h}(x,\xi) \hat{\psi}_H(x,\xi) + \frac{1}{2} \int dy V(x,\xi;y,\xi) \hat{\psi}_H(y,\xi) \hat{\psi}_H(x,\xi) - \frac{1}{2} \int dy V(y,\xi;x,\xi) \hat{\psi}_H(x,\xi) \hat{\psi}_H(y,\xi) \hat{\psi}_H(x,\xi) = \hat{h}(x,\xi) \hat{\psi}_H(x,\xi) + \int dy V(x,\xi;y,\xi) \hat{\psi}_H(y,\xi) \hat{\psi}_H(x,\xi).
\]
The third line is obtained because of the symmetry properties of \( V \)
\[
V(x,\xi;y,\xi) = V(y,\xi;x,\xi).
\]  
(H.19)
Recalling the definition of the mixed Green’s function $G(11')$ in equation (H.15) and using the relationship derived above, one finds the mixed equation of motion on contour $C$ from Figure H.1

$$\left( i\hbar \frac{d}{d\xi} + \hat{h}(1) \right) G(11') = \delta(11') - i\hbar \int_C d2 \mathcal{V}(12) G^{(2)}(12'1'), \quad (H.20)$$

where

$$\mathcal{V}(12) = V(x_1, \xi_1; x_2, \xi_2) \delta(\xi_1 - \xi_2), \quad (H.21)$$

and

$$G^{(2)}(12'1') = \left( \frac{i}{\hbar} \right)^2 \langle T_C \{ \hat{\psi}_H(1) \hat{\psi}^\dagger_H(2) \hat{\psi}_H(2') \hat{\psi}^\dagger_H(1') \} \rangle. \quad (H.22)$$

As for the real-time Green’s function $G(11')$, one can introduce a self-energy $\Sigma(11')$ for the mixed $G(11')$. It is given by

$$\Sigma(11') = -i\hbar \int_C d2 \int_C d3 \mathcal{V}(12) G^{(2)}(1232) G^{-1}(31'). \quad (H.23)$$

To find analytical expressions for $\Sigma(11')$, the same procedure as described in Appendix F can be used. Furthermore, the inverse mixed free Green’s function $G^{-1}_0(12)$ corresponding to equation (2.10) is defined as

$$G^{-1}_0(12) = \left( i\hbar \frac{d}{d\xi} + \hat{h}(1) \right) \delta(12). \quad (H.24)$$

### H.3 Dyson Equation on the Extended Contour

Collecting all the previous equations, one sees that the mixed Green’s function $G(11')$ satisfies the Dyson equation on the extended contour $C$ (Figure H.1). This equation and its adjoint can be written in the form

$$\int_C d2 G^{-1}_0(12) G(21') = \delta(11') + \int_C d2 \Sigma(12) G(21')$$

$$\int_C d2 G(12) G^{-1}(21') = \delta(11') + \int_C d2 G(12) \Sigma(21'). \quad (H.25)$$

The difference between the mixed Green’s functions $G(11')$ and the usual real-time (on part $C$ of the contour $C$) and thermodynamic Green’s functions (on part $C_\tau$ of $C$) is conveniently illustrated by expressing $G(11')$ in terms of its components. With the definition of the contour $C$ from Figure H.1, one writes

$$G(11') = \begin{cases} G(11') = -\frac{i}{\hbar} \left( T \{ \hat{\psi}_H(1) \hat{\psi}^\dagger_H(1') \} \right), & 1,1’ \text{ on } C, \\ G^>(11') = -\frac{i}{\hbar} \left( \hat{\psi}_H(1) \hat{\psi}^\dagger_H(1') \right), & 1 \text{ on } C, 1’ \text{ on } C, \\ G^<(11') = \frac{i}{\hbar} \left( \hat{\psi}_H(1') \hat{\psi}_H(1) \right), & 1 \text{ on } C, 1’ \text{ on } C_\tau, \\ i\pi G(11') = -\frac{i}{\hbar} \left( T_\tau \{ \hat{\psi}_H(1) \hat{\psi}^\dagger_H(1') \} \right), & 1,1’ \text{ on } C_\tau, \end{cases} \quad (H.26)$$
where $G(1')$ and $G(1)$ are the real-time Green’s function form equation (1.41) and the thermodynamic Green’s function from (1.11), respectively. One also has to consider the “cross Green’s functions” $G^<(1')$ and $G^>(1')$, which are constructed from Heisenberg operators with different types of evolution. These functions satisfy the obvious boundary conditions

$$
G^<(1')|_{t'=t_0} = \frac{i\hbar}{\lambda}G(1')|_{t'=0}, \quad G^<(1')|_{t=t_0} = \frac{i\hbar}{\lambda}G(1')|_{t=0},
$$

and

$$
G^>(1')|_{t'=t_0} = G^>(1')|_{t=t_0}, \quad G^<(1')|_{t'=0} = G^<(1')|_{t=0},
$$

which relate them to the thermodynamic and real-time Green’s functions. Secondly, the operator $G_0^{-1}(1')$ from equation (H.24) is defined as

$$
G_0^{-1}(1') = \begin{cases} 
G_0^{-1}(1') = \left( i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) \delta(t, t') \delta(x - x'), & 1,1' \text{ on } C \\
-\i\hbar G_0^{-1}(1') = \i\hbar \left( \frac{d}{dt} + \lambda^{(1)}(x) \right) \delta(t - t') \delta(x - x'), & 1,1' \text{ on } C_t \\
0, & \text{otherwise.}
\end{cases}
$$

Finally, the components of the self-energy $\Sigma(1')$ from equation (H.23) will be denoted by

$$
\Sigma(1') = \begin{cases} 
\Sigma(1'), & 1,1' \text{ on } C \\
K^<(1'), & 1 \text{ on } C, 1' \text{ on } C_t \\
K^>(1'), & 1 \text{ on } C_t, 1' \text{ on } C \\
-\i\hbar K(1'), & 1,1' \text{ on } C_t
\end{cases}
$$

where $\Sigma(1')$ contains $\Sigma^< (1')$ and $\Sigma^{R,A} (1')$.

### 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 $C$ from Figure H.1, one has, since the part $C_r$ is later along $C$ than $C$ (only the first equation will be considered for each case)

$$
\left( i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G(1') = \delta(1') + \int_C d2 \Sigma(12) G(21') + \int_{C_r} d2 \mathcal{K}^<(12) G^>(21').
$$

Recalling the Langreth theorem from section 2.3, one obtains for the different components of $G(1')$

$$
\left( i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G^<(1') = \int_{t_0}^\infty d2 \Sigma^{R}(12) G^>(21') + \int_{t_0}^\infty d2 \Sigma^{<}(12) G^A(21')
$$

and

$$
\left( i\hbar \frac{d}{dt} + \frac{\hbar^2 \nabla_1^2}{2m} \right) G^{R,A}(1') = \int_{t_0}^\infty d2 \Sigma^{R,A}(12) G^{R,A}(21').
$$
with \( \int_0^\infty d2 = \int_0^\infty dt_2 \int dx_2 \).

It is obvious that the integration over \( C_r \) 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 \( C_r \) of the contour \( C \) (Figure H.1). Thus one arrives at equation

\[
\int_{C_r} d2 \left( G_0^{-1}(12) - \mathcal{K}(12) \right) G(21') = \delta(11') + \int_{C_r} d2 \mathcal{K}^>(12) G^<(21') - \int_{C_r} d2 \mathcal{K}^>(12) G^<_(21')
\]

\[
= \delta(11') + \int_0^\infty d2 \mathcal{K}^>(12) G^<_(21')
\]

\[
= \delta(11') \quad \text{(H.30)}
\]

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 \( G^<_(21') \) 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 \( G(11') \) 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 \( G(11') \), one derives the equations of motion for the cross components \( G^<_R \). In equation (H.25), 1 is now on the \( C \) part of the contour \( C \) and 1’ on \( C_r \). Hence one obtains

\[
\int_{C_r} d2 \left( G_0^{-1}(12) - \Sigma(12) \right) G^<_R(21') = \frac{i}{\hbar} \int_{C_r} d2 \mathcal{K}^<_R(12)G^<_R(21').
\]

(H.31)

With the definitions of \( \Sigma(12) \) given in [11]

\[
\Sigma(12) = \Sigma^\delta + \theta(t_1, t_2) \Sigma^>(12) + \theta(t_2, t_1) \Sigma^<(12)
\]

\[
\Sigma^R(12) = \Sigma^\delta + \theta(t_1 - t_2) \left( \Sigma^>(12) - \Sigma^<_R(12) \right),
\]

where \( \Sigma^\delta \) 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

\[
\int_{C_r} d2 G_0^{-1}(12) G^<_R(21') = \int_0^\infty d2 \Sigma^R(12) G^<_R(21') + \frac{i}{\hbar} \int_{C_r} d2 \mathcal{K}^<_R(12)G^<_R(21').
\]

This equation describes the evolution of \( G^<_R(11') = G^<_R(x, t; x', \tau') \) with respect to its real-time argument \( t \). To derive the equation describing the imaginary evolution
of $\mathcal{G}^{\leq}(11')$, one uses the second equation in (H.25), still with 1 on the $C$ part of the contour $C$ and $1'$ on $C_{\tau}$

$$\int_{C_{\tau}} d^{2} \mathcal{G}^{\leq}(12) \left( \mathcal{G}_0^{-1}(21') - \mathcal{K}(21') \right) = \frac{i}{\hbar} \int_{t_0}^{\infty} d^{2} \mathcal{G}^R(12) \mathcal{K}^{\leq}(21'). \quad (H.32)$$

The analogous procedure can be repeated for $\mathcal{G}^{\geq}(11')$. The results are given in [22].
Bibliography


