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MANY-BODY APPROACH TO TIME-DEPENDENT QUANTUM TRANSPORT

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Abstract

In this thesis the electron transport through interacting quantum wires is studied. The time-dependent properties of the system are investigated by using the non-equilibrium Green function technique. This technique provides a way to include ultra-fast time-dependent processes, arbitrary strong external fields and also brings forward an effective treatment of electron-electron and electron-phonon interactions. The electron-electron interactions are included via various self-energy approximations at Hartree-Fock, second-order Born and GW levels. These approximations are called conserving since they fulfill the physical conservation laws like the charge conservation law. The interacting central system is coupled to one-dimensional tight-binding leads, which are considered effectively as noninteracting. The system is perturbed by a bias voltage after which the time-evolution of the system is followed by Kadanoff-Baym equations. The non-equilibrium steady-state value of the current depends on the used self-energy approximation, which indicates the importance of the history-dependence in the calculation of current. This is an important observation in the aspect of time-dependent density functional theory, since it is one indication for the need of functionals with memory. The steady-state current is independent of the initial state, which is in accordance with the memory-loss theorem. The transient current shows small oscillations, which are consequence of the density oscillations especially in the first and last site. The density oscillations in the sites are effect of the electron transition from the lead to the central system and vice versa.

Tiivistelmä

Työssä tutkitaan varauskuljetusilmiöitä vuorovaikuttavien kvanttisysteemien lävitse käyttäen epätasapainon Greenin funktio teoriaa. Epätasapainon Greenin funktio teorian etuna on, että sen avulla voidaan tarkastella nopeasti ajan funktiona muuttuvia ilmiöitä ja suuria ulkoisia kenttiä. Lisäksi elektroni-elektroni sekä elektroni-fononi vuorovaikutukset on mahdollista käsitellä tehokkaasti itseisenergioita käyttäen. Tässä työssä elektroni-elektroni vuorovaikutukset huomioidaan Hartree-Fock, toisenasteen Bornin ja *GW* approksimaatioiden tasoilla. Kaikki nämä approksimaatiot ovat fysikaaliset säilymislait toteuttavia. Epätasapainon Greenin funktio menetelmää käyttäen lasketaan virta vuorovaikuttavien mallikvanttisysteemien lävitse, jotka ovat kytketty efektiivisesti vuorovaikuttamattomiin yksidimensioanaalisiin tiukansidoksenmallilla kuvattuihin joh-timiin. Systeemi ajetaan epätasapainoon ulkoisen jännitteen avulla, jonka jälkeen systeemin aikaevoluutiota seurataan Kadanoff-Baym yhtälöitä käyttäen. Valitulla itseis-energia-approksimaatiolla on vaikutus tasapainovirran suuruuteen, joka osoittaa historiariippuvuuden tärkeyden tarkastellussa systeemissä. Tämä on tärkeä huomio, jos halutaan käyttää ajasta riippuvaa tiheysfunktionaaliteoriaa, jolloin funktionaalien muistiominaisuudet tulevat tärkeiksi. Tasapainovirta on riippumaton alkutilasta mikä on konsistenttia *memory-loss*-teoreeman kanssa. Toisaalta alkutila vaikuttaa hetkelliseen virtaan ennen tasapainotilan kehittymistä. Virrassa havaitaan pientä oskillaatiota heti jännitteen kytkemisen jälkeen mikä on seurasta tiheyden oskillaatioista etenkin ensimmäisessä ja viimeisessä ketjun mallimolekyylissä. Tämä tiheysoskillaatio on puolestaan seurasta elektronien siirtymisestä johtimesta keskuskappaleeseen ja päinvastoin.

Contents

1 Introduction

A study of quantum transport has gained an increasing amount of interest during the last years. The succeeded measurements of conductance through single molecules and increased computational power, implying more accurate and realistic simulations, are part of the reason for enthusiasm towards quantum transport and molecular electronics [1–4]. The transport problem through a single molecule is a non-equilibrium process where the electron-electron interactions, fast time-dependence and strong external fields play a major role. Studying charge transport through a molecule, description of the electronic structure properly, at least for the parts which engage in the transport process, is obviously crucial when describing realistic systems. Availability of unoccupied states inside the bias window is essential for having any decent transmission through the system.

Coupling of the molecule to the macroscopic leads and applying an external field modifies the electronic states of the central molecule. The electronic states of the central molecule are described by the spectral function, which gives the occupation probability distribution of the quasiparticles. In the weak-coupling regime one could identify distinct quasiparticle states and effectively the system can be treated as weakly interacting and the Hartree-Fock approximation gives sufficient results. Interactions between electrons in the molecule and in the leads play a bigger role when the coupling is strong since the electrons can move easier from electrodes to the central molecule and backwards. Interactions in the leads can also affect to the current since the applied bias voltage will drive the electrons towards the "bottle neck" where the electron correlation is big.

There are basically two methods to tackle the problem of time-dependent quantum transport for bigger systems than Anderson impurity model. One is time-dependent density functional theory and another is non-equilibrium Green function method. The density functional theory has nevertheless a weakness, namely a lack of suitable functionals. The known functionals describe only static density distributions which is not true any more in the transport problem. The non-equilibrium Green function technique offers a way to treat the non-equilibrium processes, the electron-electron interactions, time-dependence and arbitrary strong external fields. The time evolution of the system is described by analytically continuating the equilibrium Green function from the imaginary axis to the real axis. This is done according to so-called Langreth rules and leads to Kadanoff-Baym equations. The electron-electron interactions are included by various selections of self-energy diagrams. The strong external field can be

treated non-perturbatively by using non-equilibrium Green function technique, since the external potential is just a parameter in the theory.

The power of Green functions is in the perturbative treatment of self-energy, which is the term containing the information of the many-particle properties of the system. The approximations of many-body interactions can be improved by taking into account those Feynman diagrams, which are relevant for the studied process. Although the Green function does not contain the full information carried by the wave function, it contains all the necessary information. For example: the expectation values of one-body operators, ionization potentials, response functions, spectral functions and total energy of the system.

The non-equilibrium Green function method provides also a way to derive new improved density functionals with memory, which can be used to study the transport problem with the time-dependent density functional theory. The construction of functionals is based on the diagrammatic expansion of Green functions. There is at least three ways to construct variational functionals form the diagrammatic expansion. First is to re normalize the Green function lines which leads to Luttinger-Ward functional, the second way is to renormalize the interaction lines which leads to Hedin-Almbladh functional. The third way is to renormalize the four-point vertex.

In this text the method for calculating the current through model system by using non-equilibrium Green function method is described. The systems we are studying consist of central transport region and two macroscopic leads to which the molecule is connected. The central system is treated as interacting whereas the leads are treated noninteracting. The effect of the leads to the central system is included in terms of embedding self-energy, which is added to the many-body self-energy approximation describing the interactions in the central system.

In first chapter the non-equilibrium Green functions and the time contour are introduced. The second chapter contains the derivation of equation for current whereas the third chapter is about the different self-energy approximations and also the description of leads is included. Chapter six is about the steady-state current and the last chapter is devoted for the results.

2 Time contour and Green functions

The non-equilibrium Green function technique provides a method to study interacting electrons at finite temperatures under an arbitrary strong time-dependent external potential. The equilibrium description of interacting many-particle systems is rather straightforward, if the interactions are turned on and off adiabatically, the ground state at the beginning and the state at the end can be assumed to be the same. The states of the interacting system, needed to obtain the Green function for interacting system, can be constructed form the eigenstates of the noninteracting system by the Gell-Mann and Low theorem [5].

In the non-equilibrium situation the ground state at $t = -\infty$ is not necessary anymore exactly the same as the state we obtain at $t = \infty$, when the interactions have been turned on and off adiabatically. Actually, it is quite easily seen that these states do not need to be identical. For example, by taking a noninteracting state at $t = -\infty$, switching on the interactions, the system being fully interacting at $t = 0$ and after switching off the interactions, the system can end up to the state which is at a different energy than the original state due to dissipative processes. As an example one could think a ferromagnetic material, which has been exposed to an external magnetic field. At first the material is unmagnetized, after applying a magnetic field the material will be magnetized even through the external magnetic field is removed. Another example is the ionization of a molecule by a laser field. In this case also the final state after the perturbation is different from the starting state, since there is a lack of one or more electrons.

2.1 Time-evolution

To be able to characterize the non-equilibrium properties of a quantum system we need to follow the time-evolution of this system. In quantum mechanics the time-evolution is given by the unitary time-evolution operator $\hat{U}(t, t')$, which, because of unitarity, leaves the observables invariant. In mathematicians language the evolution operator is a mapping between the wave functions at times t and t' i.e.

$$|\Psi(t)\rangle = \hat{U}(t, t')|\Psi(t')\rangle. \tag{2.1}$$

A formal solution for this equation can be found by differentiating with respect to t and t' and by using the time-dependent Schrödinger equation. The evolution operator

is defined as a solution of following differential equations with the boundary condition $\hat{U}(t,t) = 1$,

$$i\partial_t \hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t'), \tag{2.2}$$

$$-i\partial_{t'} \hat{U}(t,t') = \hat{H}(t')\hat{U}(t,t'). \tag{2.3}$$

Solving, for example, the first equation by integration from t' to t with the boundary condition a following equation for $\hat{U}(t,t')$ is obtained

$$\hat{U}(t,t') = 1 - i\int_{t'}^{t} \mathrm{d}\tilde{t}\, \hat{H}(\tilde{t})\hat{U}(\tilde{t},t'). \tag{2.4}$$

This equation will give successive approximations for the time-evolution for operator. For example

$$\begin{aligned}
\hat{U}_0(t,t') &= 1 \\
\hat{U}_1(t,t') &= 1 - i\int_{t'}^{t} dt_1 \hat{H}(t_1) \\
\hat{U}_2(t,t') &= 1 - i\int_{t'}^{t} dt_1 \hat{H}(t_1) + (-i)^2 \int_{t'}^{t} dt_1 \hat{H}(t_1) \int_{t'}^{t_1} dt_1 dt_2 \hat{H}(t_2).
\end{aligned} \tag{2.5}$$

By repeated use of equation (2.4) one ends up to the following N-th order approximation for $\hat{U}(t,t')$

$$\hat{U}_N(t,t') = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} \mathrm{d}\tilde{t}_1 \int_{t'}^{t} \mathrm{d}\tilde{t}_2 \ldots \int_{t'}^{t} \mathrm{d}\tilde{t}_n\, \mathcal{T}[\hat{H}(\tilde{t}_1)\ldots\hat{H}(\tilde{t}_n)]. \tag{2.6}$$

A similar equation can also be derived for the adjoint equation (2.3). The result is

$$\hat{U}_N(t,t') = 1 + \sum_{n=1}^{\infty} \frac{i^n}{n!} \int_{t}^{t'} \mathrm{d}\tilde{t}_1 \int_{t}^{t'} \mathrm{d}\tilde{t}_2 \ldots \int_{t}^{t'} \mathrm{d}\tilde{t}_n\, \tilde{\mathcal{T}}[\hat{H}(\tilde{t}_1)\ldots\hat{H}(\tilde{t}_n)]. \tag{2.7}$$

These two equations can be written formally as [6, 7]

$$\begin{aligned}
\hat{U}(t,t') &= \mathcal{T}\left[\exp\left(-i\int_{t'}^{t} \mathrm{d}\tau\, \hat{H}(\tau)\right)\right], \quad \text{if } t' < t, \\
\hat{U}(t,t') &= \tilde{\mathcal{T}}\left[\exp\left(i\int_{t}^{t'} \mathrm{d}\tau\, \hat{H}(\tau)\right)\right], \quad \text{if } t' > t.
\end{aligned} \tag{2.8}$$

These equations are central for the perturbation calculations of many-particle systems. The operator $\mathcal{T}$ is the time-ordering operator, which rearranges the operators

in chronological order; $\tilde{\mathcal{T}}$ is the anti-chronological time-ordering operator. The definition for $\mathcal{T}$ is

$$\mathcal{T}_C\left[\hat{A}(t_1)...\hat{A}(t_n)\right] = \sum_P (-1)^{F_p}\theta(t_{P(1)},t_{P(2)})...\theta(t_{P(n-1)},t_{P(n)}) \times \hat{A}(t_{P(1)})...\hat{A}(t_{P(n)}) \tag{2.9}$$

where P runs over permutations and F_p denotes the fermionic permutations.

In addition, for knowing how the non-equilibrium system evolves in time we need to know how to calculate the expectation values of operators in interest. From the knowledge of the density matrix in any representation it is possible to determine the expectation value of an operator $\hat{O}(t)$ in the grand canonical ensemble as

$$\langle\hat{O}(t)\rangle = \mathrm{Tr}\left\{\hat{\rho}\hat{O}_H(t)\right\}, \tag{2.10}$$

where the statistical operator $\hat{\rho}$, acting as a weight function, is defined as

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\right\}} \tag{2.11}$$

and

$$\hat{O}_H(t) = \hat{U}(t_0,t)\hat{O}\hat{U}(t,t_0) \tag{2.12}$$

is the Heisenberg-representation of an operator.

Defining the one-body part of the Hamiltonian without the coulomb-interaction to be

$$\hat{h}(\mathbf{r}t) = \frac{1}{2}\nabla^2 + v(\mathbf{r}t) - \mu \tag{2.13}$$

then the statistical operator can be written as

$$\hat{\rho}_0 = \frac{e^{-\beta\hat{H}-\mu\hat{N}}}{\mathrm{Tr}\left\{e^{-\beta\hat{H}-\mu\hat{N}}\right\}} = \frac{e^{-\beta\hat{H}_0}}{\mathrm{Tr}\left\{e^{-\beta\hat{H}_0}\right\}}, \tag{2.14}$$

where, because the number operator $\hat{N}$ and Hamiltonian commute, the term $\mu\hat{N}$ is merged to the definition of $\hat{H}_0$ ($\hat{H}_0 = \hat{H} - \mu\hat{N}$). The operator $\hat{N}$ can be replaced by the eigenvalue N only for systems of fixed particle number. For systems where the creation and annihilation of particles happens the trance in the denominator needs the be calculated over the matrix elements of $\exp[-\beta(\hat{H} - \mu\hat{N})]$ calculated with states of the Fock space, and therefore involves states with different numbers of particles.

The operator $e^{-\beta\hat{H}_0}$ can be written as an evolution operator in the imaginary time and therefore the expectation value $\langle\hat{O}(t)\rangle$ gets a following form

$$\langle\hat{O}(t)\rangle = \frac{\mathrm{Tr}\{\hat{U}(t_0-i\beta,t_0)\hat{O}_H(t)\}}{\mathrm{Tr}\{\hat{U}(t_0-i\beta,t_0)\}} = \frac{\mathrm{Tr}\{\hat{U}(t_0-i\beta,t_0)\hat{U}(t_0,t)\hat{O}\hat{U}(t,t_0)\}}{\mathrm{Tr}\{\hat{U}(t_0-i\beta,t_0)\}}. \tag{2.15}$$

From this expression it is seen that the system evolves first from an initial time $(t_0, 0)$ to a time $(t, 0)$, the operator $\hat{O}$ acts and the system evolves back to time $(t_0, 0)$ from where the system is evolving along the imaginary track to the time $(t_0, -i\beta)$. This time-contour in the complex t-plane (see Fig. 2.1) was originally introduced by Keldysh [8]. Because of the group property of the time-evolution operator the time contour can be expanded up to the infinity. Times are ordered on the contour such a way that t_+ is later that t_- [6, 7].

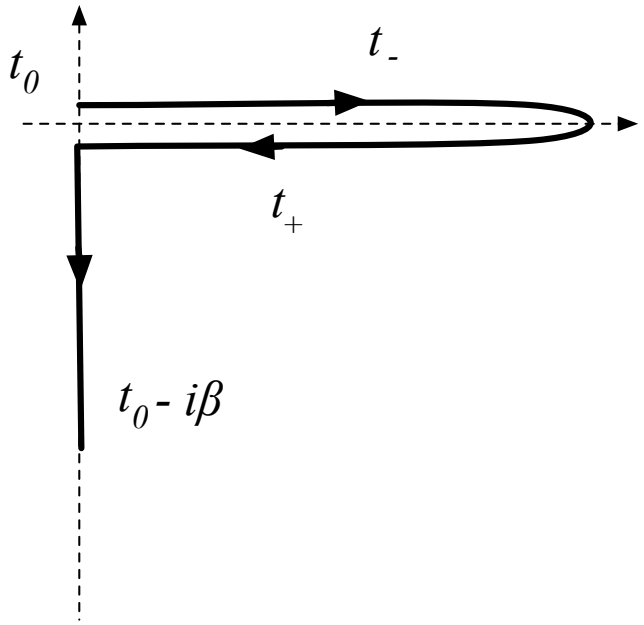

Figure 2.1: Keldysh contour.

The expectation value of an operator $\hat{O}$ can be generalized to apply on the whole contour. If z is a variable on the contour γ then after using exponent expression for the evolution operator we can formally write

$$\langle \hat{O}(z) \rangle = \frac{\mathrm{Tr}\left\{ \left[\mathcal{T} \exp\left(-i \int_\gamma d\tilde{z} \hat{H}(\tilde{z}) \right) \right] \hat{O}(z) \right\}}{\mathrm{Tr}\left\{ \mathcal{T} \exp\left(-i \int_\gamma d\tilde{z} \hat{H}(\tilde{z}) \right) \right\}}. \tag{2.16}$$

If the Hamiltonian is time-independent this expression simplifies to the ground state expectation value.

2.2 Green functions

We are now ready to define the non-equilibrium Green function

$$G(1,2) \equiv -i\langle \mathcal{T}_{\mathcal{C}}[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)]\rangle = -i\frac{\mathrm{Tr}\{\hat{U}(t_0 - i\beta, t_0)\mathcal{T}_{\mathcal{C}}[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)]\}}{\mathrm{Tr}\{\hat{U}(t_0 - i\beta, t_0)\}}, \tag{2.17}$$

where $\mathcal{T}_{\mathcal{C}}$ denotes the time ordering operator along the contour γ where the average is taken over the grand canonical ensemble. The Green function is thus defined for time arguments on the contour. If the real axis is not included to the range where the Green function is defined, *i.e.*, the Green function is defined only on the imaginary axis, this formalism reduces to the basic theory of ground state Green functions [5].

The Green function posses some symmetry relations on the imaginary track. The fermion (boson) Green function is antisymmetric (symmetric) under the change of its time arguments. These periodic Kubo-Martin-Schwinger boundary conditions are

$$\begin{aligned} G\left(\mathbf{x}_1(t_0 - i\beta), 2\right) &= -G\left(\mathbf{x}_1 t_0, 2\right), \\ G\left(1, \mathbf{x}_2(t_0 - i\beta)\right) &= -G\left(1, \mathbf{x}_2 t_0\right). \end{aligned} \tag{2.18}$$

To find a physical meaning for the Green function we write the time-ordering operator explicitly. The Green function splits into two contour ordered Green functions called the greater Green function $G^>$ and the lesser Green function $G^<$ as[6, 7]

$$G(1,2) = \theta(t_1, t_2)G^>(1,2) + \theta(t_2, t_1)G^<(1,2). \tag{2.19}$$

The step-functions are defined on the Keldysh-contour so that

$$\theta(t, t') = \begin{cases} 1, & \text{if } t_1 \text{ is later than } t_2 \\ 0, & \text{otherwise.} \end{cases} \tag{2.20}$$

The contour ordered greater and lesser correlation functions, $G^{\gtrless}(1,2)$, are defined as

$$\begin{aligned} G^>(1,2) &= -i\langle \hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\rangle, \;\; t_1 \text{ later than } t_2, \\ G^<(1,2) &= i\langle \hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\rangle, \;\; t_2 \text{ later than } t_1. \end{aligned} \tag{2.21}$$

The greater Green function $G^>(1,2)$ can be interpreted as a propagation of a particle, since we are removing a particle at point 1 and placing it at the point 2. The lesser Green function $G^<(1,2)$ describes a propagation of hole or a particle backwards in time, since we are removing a particle at later time point 1 and placing it at earlier time 2. The greater and lesser Green functions are connected via following symmetry relations

$$G^{\gtrless}(1,2) = -\left[G^{\gtrless}(1,2)\right]^*, \tag{2.22}$$

$$G^>(\mathbf{x}_1 t, \mathbf{x}_2 t) = -i\delta(\mathbf{x}_1 - \mathbf{x}_2) + G^<(\mathbf{x}_1 t, \mathbf{x}_2 t). \tag{2.23}$$

The retarded and advanced Green functions are defined as a expectation value of the anticommutator of the two field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$

$$\begin{aligned} G^R(1,2) &= -i\theta(t_1-t_2)\left\langle\left\{\hat{\psi}_H(1),\hat{\psi}_H^\dagger(2)\right\}\right\rangle \\ &= \theta(t_1-t_2)\left[G^>(1,2)-G^<(1,2)\right], \qquad (2.24) \\ G^A(1,2) &= i\theta(t_2-t_1)\left\langle\left\{\hat{\psi}_H(1),\hat{\psi}_H^\dagger(2)\right\}\right\rangle \\ &= \theta(t_2-t_1)\left[G^<(1,2)-G^>(1,2)\right], \qquad (2.25) \end{aligned}$$

where $\theta(t_2-t_1)$ is the usual Heaviside step-function. The retarded and advanced Green functions are analytic in the upper and lower half-plane respectively which is why these functions became useful in calculation of the response properties for the given system.

In addition, we can define the mixed Green functions whose one time argument is defined on the real-axis and other on the imaginary-axis

$$\begin{aligned} G^\rceil(\mathbf{x_1}t_1,\mathbf{x}_2\tau_2) &= G^<(\mathbf{x_1}t_1,\mathbf{x}_2t_0-i\tau_2), \qquad (2.26) \\ G^\lceil(\mathbf{x_1}\tau_1,\mathbf{x}_2t_2) &= G^>(\mathbf{x_1}t_0-i\tau_1,\mathbf{x}_2t_2). \qquad (2.27) \end{aligned}$$

The matsubara component of the Green function is defined purely on the imaginary axis

$$G^M(\mathbf{x_1}\tau_1,\mathbf{x}_2\tau_2) = G(\mathbf{x_1}t_0-i\tau_1,\mathbf{x}_2t_0-i\tau_2). \qquad (2.28)$$

Although, the Green function does not contain the full information carried by the wave function, it contains, nevertheless, all the necessary statistical and dynamical information like the ground state properties (expectation values) and ionization energies. The expectation value of the one-body operator $\hat{O}(\mathbf{x}t)$ is generally given by

$$\begin{aligned} \langle\hat{O}(t_1)\rangle &= \int \mathrm{d}\mathbf{x}_1 \left[\hat{O}(\mathbf{x}_2t_1)\langle\hat{\psi}_H(\mathbf{x}_1t_1)\hat{\psi}_H^\dagger(\mathbf{x}_2t_2)\rangle\right]_{\mathbf{x}_1=\mathbf{x}_2} \\ &= -i\int \mathrm{d}\mathbf{x}_1 \left[\hat{O}(\mathbf{x}_2t_1)G^<(\mathbf{x}_1t_1,\mathbf{x}_2t_1)\right]_{\mathbf{x}_1=\mathbf{x}_2}. \end{aligned} \qquad (2.29)$$

For example the particle and current are given by

$$\begin{aligned} \langle\hat{n}(1)\rangle &= -iG^(1,1^+), \\ \langle\mathbf{j}(1)\rangle &= -i\left\{\left[\frac{\nabla_1}{2i}-\frac{\nabla_2}{2i}\right]G(1,2)\right\}_{1=2^+}, \end{aligned} \qquad (2.30)$$

where the notation $^+$ means that in the time-contour t^+ approaches t from infinitesimally later time, $t^+ = t+\delta$.

2.3 Spectral function

The spectral function provides information of the correlated quasiparticle (single-particle) spectrum of the system and it can be obtained as a Fourier-transform of the Green function. The spectral function is usually defined as the difference between the greater and lesser Green funcion

$$A(\mathbf{k},\omega) = i\left[G^{>}(\mathbf{k},\omega) - G^{<}(\mathbf{k},\omega)\right]. \tag{2.31}$$

In the equilibrium Green function formalism the Hamiltonian is usually time independent which allows us to determine the Lehmann representation of the Green function [5, 9] and to Fourier-transform the Green function into the frequency domain. In the non-equilibrium situation this is not in general possible, since the Green function depends on two time arguments. Nevertheless, if in the long-time limit the Green function does not depend upon the time arguments t_1 and t_2 separately but rather on their difference $t_1 - t_2$, *i.e.* the system has reached a non-equilibrium steady state, the Green function can be Fourier-transformed to obtain the removal and addition energies of the system [6, 7].

Let us start by expressing the Green function on the frequency domain as

$$\begin{aligned} G(\mathbf{x}_1,\mathbf{x}_2;\omega) &= \int d\tau G(\mathbf{x}_1,\mathbf{x}_2;\tau)e^{-i\omega\tau} \\ &= \int \mathrm{d}(t_2-t_1)\theta(t_1,t_2)G^{>}(\mathbf{x}_1,\mathbf{x}_2;t_2-t_1)e^{-i\omega(t_2-t_1)} \\ &+ \int \mathrm{d}(t_2-t_1)\theta(t_2,t_1)G^{<}(\mathbf{x}_1,\mathbf{x}_2;t_2-t_1)e^{-i\omega(t_2-t_1)}. \end{aligned} \tag{2.32}$$

We can formally calculate this by using the complete eigenstates of the Hamiltonian and obtain the Lehman-representation of the greater and lesser Green function. From the definition of the greater Green function we get

$$\begin{aligned} G^{>}(\mathbf{x}_1t_1,\mathbf{x}_2t_2) &= -i\,\mathrm{Tr}\left\{\hat{\rho}_0\,\hat{\psi}(\mathbf{x}_1t_1)\hat{\psi}^{\dagger}(\mathbf{x}_2t_2)\right\} \\ &= \sum_i \langle\phi_i|\hat{\rho}_0\,\hat{\psi}(\mathbf{x}_1t_1)\hat{\psi}^{\dagger}(\mathbf{x}_2t_2)|\phi_i\rangle \end{aligned} \tag{2.33}$$

and by inserting a complete set of eigenstates between the field operators we obtain

$$G^{>}(\mathbf{x}_1t_1,\mathbf{x}_2t_2) = -\frac{i}{Z}\Big[\sum_{ij} e^{-\beta E_i}e^{i(E_j-E_i)(t_2-t_1)}\langle\phi_i|\hat{\psi}(\mathbf{x}_1)|\phi_j\rangle\langle\phi_j|\hat{\psi}^{\dagger}(\mathbf{x}_2)|\phi_i\rangle\Big], \tag{2.34}$$

where $Z = \mathrm{Tr}[e^{\beta H}] = \mathrm{Tr}[\hat{U}(t_0 - i\beta, t_0)]$ is the grand partition function. A similar analysis for the lesser Green function gives

$$G^{<}(\mathbf{x}_1t_1,\mathbf{x}_2t_2) = \frac{i}{Z}\Big[\sum_{ij} e^{-\beta E_i}e^{i(E_i-E_j)(t_2-t_1)}\langle\phi_i|\hat{\psi}^{\dagger}(\mathbf{x}_2)|\phi_j\rangle\langle\phi_j|\hat{\psi}(\mathbf{x}_1)|\phi_i\rangle\Big]. \tag{2.35}$$

The states ϕ_j contain $N \pm 1$ particles if the state ϕ_i contains N particles. This is seen easily as follows. The commutator of the number operator with the field operator is $\left[\hat{N}_\alpha(1), \hat{\psi}_\beta(2)\right] = -\hat{\psi}_\beta(2)$ or equivalently $\hat{N}_\alpha(1)\hat{\psi}_\beta(2) = \hat{\psi}_\beta(2)[\hat{N} - 1]$. Applying this operator to the state $|\phi_i\rangle$ gives $\hat{N}(1)[\hat{\psi}(2)|\phi_i\rangle] = [N-1][\hat{\psi}(2)|\phi_0\rangle]$, therefore the state $|\phi_i\rangle$ has N particles [5]. We can now write the equations (2.34) and (2.35) as follows

$$G^<(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2) = \frac{i}{Z}\sum_{ij} e^{-\beta E_i} e^{i(E_i - E_j)(t_2 - t_1)} g^*_{ij}(\mathbf{x}_2) g_{ji}(\mathbf{x}_1), \tag{2.36}$$

$$G^>(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2) = -\frac{i}{Z}\sum_{ij} e^{-\beta E_i} e^{i(E_j - E_i)(t_2 - t_1)} f_{ij}(\mathbf{x}_1) f^*_{ji}(\mathbf{x}_2), \tag{2.37}$$

where we have also introduced the Feynman-Dyson amplitudes for a simplification of the notation

$$g_{ji}(\mathbf{x}_1) = \langle N-1, j|\hat{\psi}(\mathbf{x}_1)|\phi_i\rangle, \tag{2.38}$$

$$f_{ij}(\mathbf{x}_1) = \langle \phi_i|\hat{\psi}(\mathbf{x}_1)|N+1, j\rangle. \tag{2.39}$$

The spectral function is defined now as a Fourier-transform of the Green function

$$A^{\gtrless}(\mathbf{x}_1, \mathbf{x}_2, \omega) = \int d(t_2 - t_1) G^{\gtrless}(\mathbf{x}_1, \mathbf{x}_2, t_2 - t_1) e^{i\omega(t_2 - t_1)} \tag{2.40}$$

and it gives the removal and addition energies of the electrons in the system

$$A^<(\mathbf{x}_1, \mathbf{x}_2, \omega) = \frac{i}{Z}\sum_{ij} \delta(\omega + E_j - E_i) e^{-\beta E_i} g^*_{ij}(\mathbf{x}_2) g_{ji}(\mathbf{x}_1), \tag{2.41}$$

$$A^>(\mathbf{x}_1, \mathbf{x}_2, \omega) = -\frac{i}{Z}\sum_{ij} \delta(\omega + E_i - E_j) e^{-\beta E_i} f_{ij}(\mathbf{x}_1) f^*_{ji}(\mathbf{x}_2). \tag{2.42}$$

The coefficients are called spectral weight functions. The spectral function gives a measure how well the system can be treated as consisting of noninteracting quasiparticles. If the system is treated as noninteracting, the spectral function is just a sum of delta functions. The interactions change profile of the spectral function from the ideal delta functions to a more broaden Lorentzian or gaussian peaks (see Fig. 2.2).

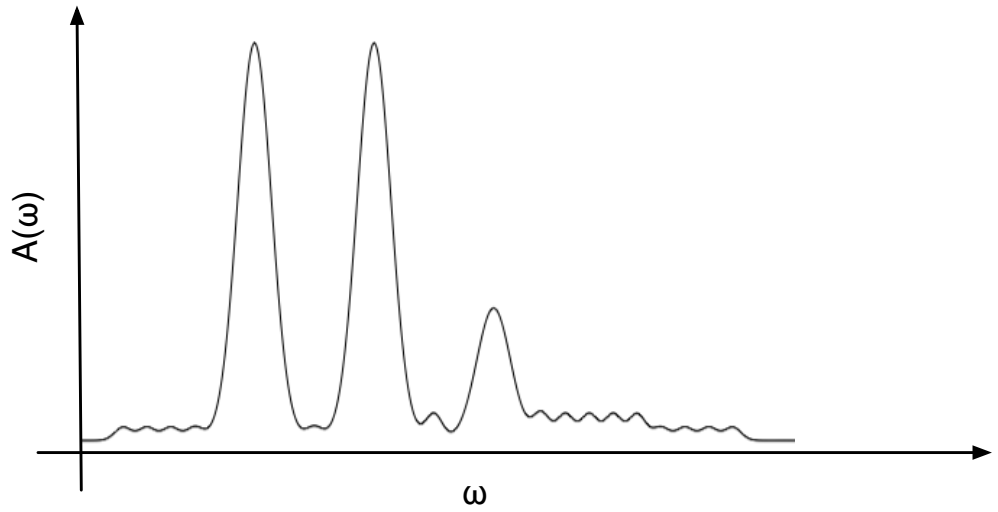

Figure 2.2: Spectral function which shows three spectral peaks and the correlated background noise.

Now we can go back to the calculation of the Fourier-transform of the total Green function (Eq. (2.32)), which can be written as

$$\begin{aligned} G(\mathbf{x}_1,\mathbf{x}_2;\omega) &= \int \mathrm{d}(t_2-t_1)\left[-\int \frac{\mathrm{d}\tilde{\omega}}{2\pi i}\frac{e^{-i\tilde{\omega}(t_1-t_2)}}{\tilde{\omega}-i\eta}\right] e^{-i\omega(t_2-t_1)} \\ &\times \left[-\frac{i}{Z}\sum_{ij} e^{-\beta E_i} e^{i(E_j-E_i)(t_2-t_1)} f_{ij}(\mathbf{x}_1) f^*_{ji}(\mathbf{x}_2)\right] \\ &+ \int \mathrm{d}(t_2-t_1)\left[-\int \frac{\mathrm{d}\tilde{\omega}}{2\pi i}\frac{e^{-i\tilde{\omega}(t_2-t_1)}}{\tilde{\omega}-i\eta}\right] e^{-i\omega(t_2-t_1)} \\ &\times \left[\frac{i}{Z}\sum_{ij} e^{-\beta E_i} e^{i(E_i-E_j)(t_2-t_1)} g^*_{ij}(\mathbf{x}_2) g_{ji}(\mathbf{x}_1)\right]. \end{aligned} \tag{2.43}$$

After some simplifications the Green function takes a following form

$$\begin{aligned} G(\mathbf{x}_1,\mathbf{x}_2;\omega) &= \frac{i}{Z}\sum_{ij}\left[\frac{e^{-\beta E_i} f_{ij}(\mathbf{x}_1) f^*_{ji}(\mathbf{x}_2)}{\omega - E_j - E_i + i\eta} + \frac{e^{-\beta E_i} g^*_{ij}(\mathbf{x}_2) g_{ij}(\mathbf{x}_1)}{\omega + E_i - E_j - i\eta}\right] \\ &= \frac{i}{Z}\int d\tilde{\omega}\left[\frac{A^{>}(\mathbf{x}_1,\mathbf{x}_2,\tilde{\omega})}{\omega+\tilde{\omega}+i\eta} + \frac{A^{<}(\mathbf{x}_1,\mathbf{x}_2,\tilde{\omega})}{\omega-\tilde{\omega}-i\eta}\right]. \end{aligned} \tag{2.44}$$

As a short summary, we have defined the Green function as an expectation value of time-ordered product of two field operators in the time contour. We were able to express the expectation value of an operator using the time-evolution operator,

which lead us to the definition of the Keldysh-contour. The Fourier-transform of the Green function allows us to determine the spectral function. The poles of the spectral function determine the allowed energies of the quasi-particles.

2.4 The equation of motion of the Green function

In order to obtain an equation for the current through the system we need to calculate the Green function. There are two ways of doing this one is the usual way by obtaining the Green function from the Hamiltonian the other way, which is also more convenient, is to use Keldysh-techniques [6, 7]. First we derive the equation of motion for the Green function describing the closed system. The equation of motion for Green function is easily found by using the Heisenberg equation of motion for time dependent operators

$$i\partial_t \hat{O}(t) = \left[\hat{O}(t), \hat{\mathrm{H}}(t)\right]. \tag{2.45}$$

The Hamiltonian can be expressed in terms of the field-operators using the language of the second-quantization as (see Appendix)

$$\begin{aligned}\hat{\mathrm{H}}(t) = &\int \mathrm{d}\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\hat{h}(\mathbf{x},t)\hat{\psi}(\mathbf{x}) \\ &+ \frac{1}{2}\int \mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2\, \hat{\psi}^\dagger(\mathbf{x}_1)\hat{\psi}^\dagger(\mathbf{x}_2)w(\mathbf{x}_1t_1,\mathbf{x}_2t_2)\hat{\psi}(\mathbf{x}_2)\hat{\psi}(\mathbf{x}_1),\end{aligned} \tag{2.46}$$

where $w(\mathbf{x}t,\mathbf{x}'t') \equiv \delta(t,t')/|\mathbf{x}-\mathbf{x}'|$ is the coulomb interaction and $\hat{h}(\mathbf{x}t)$ is the one-body Hamiltonian. By using the commutator relation of field operator $\hat{\psi}$ with Hamiltonian $\hat{\mathrm{H}}$

$$i\partial_{t_1}\hat{\psi}(1) = \left[\hat{\psi}(1), \hat{\mathrm{H}}(1)\right] = \hat{h}(1)\hat{\psi}(1) + \int \mathrm{d}2\; w(1,2)\hat{\psi}^\dagger(2)\hat{\psi}(2)\hat{\psi}(1) \tag{2.47}$$

one can obtain a following equation of motion for the Green function

$$\begin{aligned}i\partial_{t_1}G(1,2) &= i\partial_{t_1}\left[\theta(t_1,t_2)\langle\hat{\psi}(1)\hat{\psi}^\dagger(2)\rangle - \theta(t_2,t_1)\langle\hat{\psi}^\dagger(2)\hat{\psi}(1)\rangle\right] \\ &= \delta(1,2) + \hat{h}(1)G(1,2) + \int \mathrm{d}3\, w(1,3)\mathcal{T}_\mathcal{C}[\hat{\psi}^\dagger(3)\hat{\psi}(3)\hat{\psi}(1)\hat{\psi}^\dagger(2)].\end{aligned} \tag{2.48}$$

The term $\mathcal{T}_\mathcal{C}[\hat{\psi}^\dagger(3)\hat{\psi}(3)\hat{\psi}(1)\hat{\psi}^\dagger(2)]$ can be identified to be the two-particle Green function $G(1,3;3^+,2)$, which describes the motion of two particle, or two holes, or a particle and a hole. The equation of motion is then

$$i\partial_{t_1}G(1,2) = \delta(1,2) + \hat{h}(1)G(1,2) - i\int \mathrm{d}3\; w(1,3)G(1,3;3^+,2). \tag{2.49}$$

From this expression it is seen that the equation of motion for single-particle Green function depends on the higher-order Green functions. By writing the equation of

motion for two-particle Green function would contain a three-particle Green function and so on. The physical reason for occurrence of $(n+1)$-particle Green function in equation of motion of n-particle Green function is that the addition and propagation of a particle creates more and more complicated interactions to the system.

To get physics out of the equation of motion the infinite sum has to be summed or truncated. The truncation can be done self-consistently by introducing a self-energy Σ such that $-iG_2w = \Sigma G$. Now the equation of motion reads as

$$[i\partial_{t_1} - \hat{h}(1)]G(1,2) = \delta(1,2) + \int \mathrm{d}3\ \Sigma(1,3)G(3,2). \tag{2.50}$$

The self-energy $\Sigma[G]$ is a functional of the Green function. Calculating the time derivative of the Green function with respect to t_2 we obtain a adjoint form of the EOM which reads as

$$[-i\partial_{t_2} - \hat{h}(2)]G(1,2) = \delta(1,2) + \int \mathrm{d}3\ G(1,3)\hat{\Sigma}(3,2). \tag{2.51}$$

The self-energy operator $\hat{\Sigma}$ is the adjoint of Σ. These two self-energy operators are same for systems initially in equilibrium, but for general initial states this is do not need to be the case [6].

3 Time-dependent current through interacting quantum system

Modeling transport process through a constriction or a molecule is a problem involving open quantum systems; quantum systems which are in a majority in nature. Using non-equilibrium Green functions as a theoretical tool for modeling the electron transport through molecular-like systems allows us to study the properties of the system which are not accessible by other means. First of all this method allows us to treat the electron-electron interactions, although perturbatively, in terms of self-energy expansions. Secondly the theory includes time-dependence and thirdly the external potential can be arbitrary strong. In this approach the system is initially in the equilibrium with common chemical potential and the system is driven out of equilibrium by applying a bias voltage.

These are major improvements towards more realistic description of transport problem and towards better understanding of open quantum systems. Other theories usually neglect the electron-electron interactions like in the scattering theory or they are concentrated on the steady state properties like Meir-Wingreen approach. Some of the previous approaches to the quantum transport problems partition the system to three different regions; left and right lead having their own chemical potentials and to the central system. At time t_0 these three parts are connected and the current flows through the system. Partitioning the system initially is purely a theoretical trick to simplify the problem, which does not give physically correct results at the transient regime. To describe these transient currents the system has to be treated as a whole and the driving perturbation is the bias voltage applied over the system.

The assumption of the noninteractiveness of the electrons can be quite drastic and misleading assumption. Since electrons are moving through a narrow system consisting few levels from which only a few are available for transport, the electron motion is correlated. Interactions in the leads are not included in our model but it is rather easy to convince himself/herself that the electrons are highly correlated at the "tip" from lead to the central region. The applied bias over the system drives the electrons towards the contacts and as a result the effect of correlations increases.

In this chapter the equation for the current through arbitrary interacting quantum system/molecule between two noninteracting leads or electron reservoirs $\{\alpha\}$ is derived. The transport problem is approached using unpartitioned scheme [10] where

the whole system is initially at thermodynamic equilibrium described by a common chemical potential μ and inverse temperature β. This derivation is based on the unpublished notes [11] by R. van Leeuwen, G. Stefanucci and P. Myöhänen.

3.1 The model system

The system consists of an interacting system connected to the noninteracting one-dimensional tight-binding leads. This system is described by the following Hamiltonian

$$\hat{\mathrm{H}}(t) = \sum_{l\sigma} \epsilon_{ll}(t)\hat{c}^\dagger_{l\sigma}\hat{c}_{l\sigma} + \sum_{k\alpha}[\epsilon_{k\alpha k\alpha} + U_\alpha(t)]\hat{c}^\dagger_{k\alpha\sigma}\hat{c}_{k\alpha\sigma} + \frac{1}{2}\sum_{ij,mn;\sigma} w_{ij,mn}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{m\sigma'}\hat{c}_{j\sigma'}\hat{c}_{n\sigma} + \sum_{lk\alpha\sigma}[V_{k\alpha,l}\hat{c}^\dagger_{k\alpha\sigma}\hat{c}_{l\sigma} + V_{l,k\alpha}\hat{c}^\dagger_{l\sigma}\hat{c}_{k\alpha\sigma}], \tag{3.1}$$

where the index α denotes the left or right lead respectively ($\alpha = L, R$), k is the index for the leads and l, i, j, m, n are indices for the central region in addition σ is the spin index. At t_0 the system is assumed to be at the thermodynamic equilibrium determined by inverse temperature β and chemical potential μ. At some time t_1 the time-dependent perturbation $U_\alpha(t)$ is switched on. In the following the diagonal terms are denoted for simplicity by one index only. The space and spin indices are also combined to one common index.

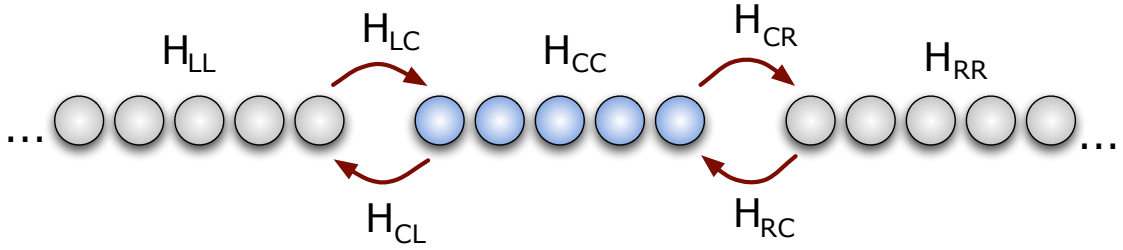

Figure 3.1: Schematic picture of the system.

Using the Hamiltonian (3.1) one can derive the equation of motion for the Green function. For that we need the following anti-commutator relations

$$\{\hat{c}_s, \hat{c}^\dagger_l\hat{c}_l\} = \hat{c}_l\delta_{sl}, \tag{3.2}$$

$$\{\hat{c}_s, \hat{c}^\dagger_i\hat{c}^\dagger_m\hat{c}_i\hat{c}_n\} = \hat{c}^\dagger_m\hat{c}_j\hat{c}_n\delta_{si} + \hat{c}^\dagger_i\hat{c}_j\hat{c}_n\delta_{sm}. \tag{3.3}$$

Calculating the commutator $[\hat{c}_s(t), H]$ and multiplying by $\hat{c}^\dagger_{l'}(t')$ we obtain

$$\begin{aligned} i\partial_t \hat{c}_l(t)\hat{c}^\dagger_{l'}(t') = \varepsilon_l \hat{c}_l(t)\hat{c}^\dagger_{l'}(t') + \sum_{k\alpha} V_{k\alpha,l}\hat{c}_{k\alpha}(t)\hat{c}^\dagger_{l'}(t') \\ + \sum_{jmn} w_{lj,mn}\hat{c}^\dagger_m \hat{c}_j(t)\hat{c}_n(t)\hat{c}^\dagger_{l'}(t'), \end{aligned} \tag{3.4}$$

from which by time-ordering and ensemble averaging we get

$$\begin{aligned} i\partial_t \left\langle \mathcal{T}_C \left[\hat{c}_l(t)\hat{c}^\dagger_{l'}(t')\right]\right\rangle = \varepsilon_l \left\langle \mathcal{T}_C \left[\hat{c}_l(t)\hat{c}^\dagger_{l'}(t')\right]\right\rangle + \sum_{k\alpha} V_{k\alpha,l} \left\langle \mathcal{T}_C \left[\hat{c}_{k\alpha}(t)\hat{c}^\dagger_{l'}(t')\right]\right\rangle \\ + \sum_{jmn} w_{lj,mn} \left\langle \mathcal{T}_C \left[\hat{c}^\dagger_m \hat{c}_j(t)\hat{c}_n(t)\hat{c}^\dagger_{l'}(t')\right]\right\rangle + i\delta(t,t'), \end{aligned} \tag{3.5}$$

where the delta function arises because the time-ordering operator does not commute with the time derivative. Formally written $[\partial_t, \mathcal{T}_C] = \delta(t,t')$. In the other words, the time-ordering operator involves step-functions and since $\partial_t \theta(t,t') = \delta(t,t')$ the interchange the derivative and step-function gives rise to a delta function.

Finally by multiplying with $-i$, identifying the Green functions and introducing the self-energy via $-iG_2 w = \Sigma[G]G$, the equation of motion for Green function $G_{ll'}$ is obtained

$$\begin{aligned} [i\partial_t - \varepsilon_l]G_{ll'}(t,t') = \delta(t,t') + \sum_{k\alpha} V_{k\alpha l} G_{k\alpha l'}(t,t') \\ + \int_\gamma d\bar{t}\Sigma_{ll''}(t,\bar{t})G_{l''l'}(\bar{t},t'). \end{aligned} \tag{3.6}$$

By checking all the combinations it is seen that the equation of motion for the Green function can be written in the following matrix form

$$[i\partial_t \mathbf{I} - \mathbf{H}(t)]\mathbf{G}(t,t') = \delta(t,t')\mathbf{I} + \int_\gamma \mathrm{d}\bar{t}\, \mathbf{\Sigma}_{\mathrm{MB}}(t,\bar{t})\mathbf{G}(\bar{t},t'), \tag{3.7}$$

where the Hamiltonian is given by Eq. (3.8) and the many-body self-energy is given by the Eq. (3.9). Variable t is defined on the contour so that $t = \mathrm{Re}[t] + i\mathrm{Im}[t]$. The integration is performed over the Keldysh-contour. The block-matrix form of the Hamiltonian is

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_{\mathrm{LL}} & \mathbf{H}_{\mathrm{LC}} & 0 \\ \mathbf{H}_{\mathrm{CL}} & \mathbf{H}_{\mathrm{CC}} & \mathbf{H}_{\mathrm{CR}} \\ 0 & \mathbf{H}_{\mathrm{RC}} & \mathbf{H}_{\mathrm{RR}} \end{pmatrix}, \tag{3.8}$$

where $\mathbf{H}_{\alpha\alpha}$ and $\mathbf{H}_{\mathrm{CC}}$ components describe the leads and the central system respectively, whereas the off-diagonal components describe the hopping between the leads and the central region. We only consider the central region as interacting whereas the

leads are effectively noninteracting. As a consequence, the many-body self-energy has non-vanishing elements only for the central region because the diagrammatic expansion starts and ends with an interaction line. Therefore the block matrix form of the self-energy is

$$\mathbf{\Sigma}_{MB} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{\Sigma}_{\mathrm{CC}} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.9}$$

3.2 Current formula

Next task is to derive an expression for the current using the Eq. (3.7). The current is proportional to the derivative of the particle density $\hat{n}(t)$, which is defined as $\hat{n}(t) = \langle\hat{\psi}^\dagger(t)\hat{\psi}(t)\rangle = -iG^<(t,t)$. The current through lead α is therefore

$$I_\alpha(t) = \frac{\mathrm{d}}{\mathrm{d}t}\hat{n}_\alpha(t) = -i\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{G}^<_{\alpha\alpha}(t,t) = -i\left[\partial_t\mathbf{G}^<(t,t') + \partial_{t'}\mathbf{G}^<(t,t')\right]_{t=t'}. \tag{3.10}$$

Because we know the Green function only on the central region we need to express the equation for the current in terms of central region indices. Let us first extract the $\alpha\alpha$ component from the equation of motion

$$\begin{aligned}\left[i\partial_t\mathbf{1} - \begin{pmatrix} \mathbf{H}_{\mathrm{LL}}(t) & \mathbf{H}_{\mathrm{LC}}(t) & 0 \\ \mathbf{H}_{\mathrm{CL}}(t) & \mathbf{H}_{\mathrm{CC}}(t) & \mathbf{H}_{\mathrm{CR}}(t) \\ 0 & \mathbf{H}_{\mathrm{RC}}(t) & \mathbf{H}_{\mathrm{RR}}(t) \end{pmatrix}\right] \begin{pmatrix} \mathbf{G}_{\mathrm{LL}}(t,t') & \mathbf{G}_{\mathrm{LC}}(t,t') & \mathbf{G}_{\mathrm{LR}}(t,t') \\ \mathbf{G}_{\mathrm{CL}}(t,t') & \mathbf{G}_{\mathrm{CC}}(t,t') & \mathbf{G}_{\mathrm{CR}}(t,t') \\ \mathbf{G}_{\mathrm{RL}}(t,t') & \mathbf{G}_{\mathrm{RC}}(t,t') & \mathbf{G}_{\mathrm{RR}}(t,t') \end{pmatrix} \\ = \delta(t,t')\mathbf{1} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & [\mathbf{\Sigma}^{\mathrm{MB}}_{\mathrm{CC}}\cdot\mathbf{G}_{\mathrm{CC}}](t,t') & 0 \\ 0 & 0 & 0 \end{pmatrix},\end{aligned} \tag{3.11}$$

where the following short hand notation is used

$$[\mathbf{\Sigma}_{\mathrm{CC}}\cdot\mathbf{G}_{\mathrm{CC}}](t,t') = \int_\gamma \mathrm{d}\bar{t}\,\mathbf{\Sigma}^{\mathrm{MB}}_{\mathrm{CC}}(t,\bar{t})\mathbf{G}_{\mathrm{CC}}(\bar{t},t'). \tag{3.12}$$

Multiplying the matrices and taking the $\alpha\alpha$-components we get

$$i\partial_t\mathbf{G}_{\alpha\alpha}(t,t') = \delta(t,t')\mathbf{1}_{\alpha\alpha} + \mathbf{H}_{\alpha\alpha}(t)\mathbf{G}_{\alpha\alpha}(t,t') + \mathbf{H}_{\alpha\mathrm{C}}(t)\mathbf{G}_{\alpha\mathrm{C}}(t,t'). \tag{3.13}$$

The lesser-component of this equation is

$$i\partial_t\mathbf{G}^<_{\alpha\alpha}(t,t') = \delta(t,t')\mathbf{1}_{\alpha\alpha} + \mathbf{H}_{\alpha\alpha}(t)\mathbf{G}^<_{\alpha\alpha}(t,t') + \mathbf{H}_{\alpha\mathrm{C}}(t)\mathbf{G}^<_{\alpha\mathrm{C}}(t,t'). \tag{3.14}$$

By doing a similar analysis also for the adjoint equation we obtain

$$i\partial_{t'}\mathbf{G}^<_{\alpha\alpha}(t,t') = -\delta(t,t')\mathbf{1}_{\alpha\alpha} - \mathbf{G}^<_{\alpha\alpha}(t,t')\mathbf{H}_{\alpha\alpha}(t') - \mathbf{G}^<_{\alpha\mathrm{C}}(t,t')\mathbf{H}_{\mathrm{C}\alpha}(t'). \tag{3.15}$$

Inserting the equations (3.14) and (3.15) to the expression of the current (Eq. (3.10)), taking the limit $t = t'$ and using relations $[\mathbf{G}^<_{\alpha\mathrm{C}}(t,t')]^* = -\mathbf{G}^<_{\mathrm{C}\alpha}(t',t)$ and $[\mathbf{H}_{\alpha\mathrm{C}}(t)]^* = \mathbf{H}_{\mathrm{C}\alpha}(t)$ gives the following current formula

$$\begin{aligned} I_\alpha(t) &= -i\left[\partial_t \mathbf{G}^<(t,t') + \partial_{t'}\mathbf{G}^<(t,t')\right]_{t=t'} \\ &= +\mathbf{G}_{\alpha\mathrm{C}}(t,t)\mathbf{H}_{\mathrm{C}\alpha}(t) + \mathbf{G}^*_{\alpha\mathrm{C}}(t,t)\mathbf{H}^*_{\mathrm{C}\alpha}(t) \\ &= 2\mathrm{Re}\left[\mathbf{G}^<_{\alpha\mathrm{C}}(t,t)\mathbf{H}_{\alpha\mathrm{C}}(t)\right] = 2\mathrm{Re}\sum_{k\in\mathrm{C}}\mathbf{G}^<_{\alpha k}(t,t)\mathbf{H}_{k\alpha}(t). \end{aligned} \tag{3.16}$$

The equation for the current is, therefore, the real part of the trace over the central system states of the product of coupling Hamiltonian and Green function over the contact

$$I_\alpha(t) = 2\mathrm{Re}\left\{\mathrm{Tr}_C[\mathbf{G}^<_{\alpha\mathrm{C}}(t,t)\mathbf{H}_{\mathrm{C}\alpha}(t)]\right\} = -2\mathrm{Re}\left\{\mathrm{Tr}_{\mathrm{C}}[\mathbf{G}^<_{\mathrm{C}\alpha}(t,t)\mathbf{H}_{\alpha\mathrm{C}}(t)]\right\}, \tag{3.17}$$

where we have also used the fact that the current is a real quantity. From this equation (Eq. (3.16)) we see that the current is proportional to the Green function $\mathbf{G}_{\alpha\mathrm{C}}$ which propagates the particle from the lead to the central region. The proportionality to the hopping term $\mathbf{H}_{\alpha\mathrm{C}}$ is also very intuitive, since in order to the current to flow electrons have to tunnel through the contact.

We have succeeded to get an equation for the current in terms of the lesser Green function and the hopping Hamiltonian between the lead α and the central region. Nevertheless, the Green function still depends on the lead indices and we need to find an expression for the $\mathbf{G}^<_{\alpha C}(t,t')$ in terms of the central region indices only. Therefore, we need to solve the equation of motion for the $\mathbf{G}^<_{\mathrm{C}\alpha}$ Green function. This is done by introducing the unconnected noninteracting lead Green function $\mathbf{g}(t,t')$ which satisfies the equation of motion for the block diagonal Hamiltonian. The equation of motion for the noninteracting unconnected Green function can be compactly written as

$$\left[i\partial_t\mathbf{1} - \mathbf{H} + \mathbf{H}_{\mathrm{off}}\right]\mathbf{g}(t,t') = \delta(t,t')\mathbf{1}, \tag{3.18}$$

where $\mathbf{H}_{off}$ denotes the off-diagonal terms of the full Hamiltonian and can be expressed as

$$H_{\mathrm{off}} = \sum_{ik}\left[H_{\alpha\mathrm{C},ki}\hat{c}^\dagger_k\hat{c}_i + H_{\mathrm{C}\alpha,ik}\hat{c}^\dagger_i\hat{c}_k\right], \tag{3.19}$$

where the indices i and k denote the basis functions in the central region and leads respectively. By using this equation and the equation of motion (Eq. (3.7)) we have

$$\begin{aligned} \int \mathrm{d}\bar{t}\,\mathbf{g}(t,\bar{t})\left[i\partial_{\bar{t}}\mathbf{I} - \mathbf{H}(\bar{t})\right]\mathbf{G}(\bar{t},t') &= \int \mathrm{d}\bar{t}\,\mathbf{g}(t,\bar{t})\delta(\bar{t},t')\mathbf{I} \\ &+ \int \mathrm{d}\bar{t}\,\mathbf{g}(t,\bar{t})\int \mathrm{d}\bar{\bar{t}}\,\mathbf{\Sigma}_{\mathrm{MB}}(\bar{t},\bar{\bar{t}})\mathbf{G}(\bar{\bar{t}},t'). \end{aligned} \tag{3.20}$$

Performing a partial integration

$$\begin{aligned}\int \mathrm{d}\bar{t}\,\mathbf{g}(t,\bar{t})\left[-i\overleftarrow{\partial}_{\bar{t}}\mathbf{I}-\mathbf{H}(\bar{t})\right]\mathbf{G}(\bar{t},t') &= \mathbf{g}(t,t')\mathbf{I}\\ &+\int \mathrm{d}\bar{t}\int \mathrm{d}\bar{\bar{t}}\,\mathbf{g}(t,\bar{t})\boldsymbol{\Sigma}_{\mathrm{MB}}(\bar{t},\bar{\bar{t}})\mathbf{G}(\bar{\bar{t}},t')\end{aligned} \tag{3.21}$$

and using equation (3.18) gives us the Dyson equation

$$\begin{aligned}\mathbf{G}(t,t') = \mathbf{g}(t,t') + \int_\gamma \mathrm{d}\bar{t}\,\mathbf{g}(t,\bar{t})\mathbf{H}_{\mathrm{off}}\mathbf{G}(\bar{t},t') + \\ \int_\gamma \mathrm{d}\bar{t}\mathrm{d}\bar{t}\,'\mathbf{g}(t,\bar{t})\boldsymbol{\Sigma}_{\mathrm{MB}}(\bar{t},\bar{t}')\mathbf{G}(\bar{t}',t').\end{aligned} \tag{3.22}$$

The Cα-component can be extracted in a same way as the $\alpha\alpha$-component were extracted from the equation of motion (3.11). The result is

$$\mathbf{G}_{\mathrm{C}\alpha}(t,t') = \int_\gamma \mathrm{d}\bar{t}\,\mathbf{G}_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}_{\alpha\alpha}(\bar{t},t'). \tag{3.23}$$

The lesser Green function can be obtained by taking the lesser part from the previous equation

$$\begin{aligned}\mathbf{G}^<_{\mathrm{C}\alpha}(t,t') = &\int_0^t \mathrm{d}\bar{t}\,\mathbf{G}^>_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}(\bar{t})\mathbf{g}^<_{\alpha\alpha}(\bar{t},t')\\ &+\int_t^{t'} \mathrm{d}\bar{t}\,\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}(\bar{t})\mathbf{g}^<_{\alpha\alpha}(\bar{t},t')\\ &+\int_{t'}^0 \mathrm{d}\bar{t}\,\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}(\bar{t})\mathbf{g}^>_{\alpha\alpha}(\bar{t},t')\\ &+\int_0^{-i\beta} \mathrm{d}\bar{\tau}\,\mathbf{G}^\rceil_{\mathrm{CC}}(t,\bar{\tau})\mathbf{H}_{\mathrm{C}\alpha}(\bar{\tau})\mathbf{g}^\lceil_{\alpha\alpha}(\bar{\tau},t').\end{aligned} \tag{3.24}$$

Gathering the similar terms

$$\begin{aligned}\mathbf{G}^<_{\mathrm{C}\alpha}(t,t') = &\int_0^t \mathrm{d}\bar{t}\,\left[\mathbf{G}^>_{\mathrm{CC}}(t,\bar{t})-\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t})\right]\mathbf{H}_{\mathrm{C}\alpha}(\bar{t})\mathbf{g}^<_{\alpha\alpha}(\bar{t},t')\\ &+\int_0^{t'} \mathrm{d}\bar{t}\,\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}(\bar{t})\left[\mathbf{g}^<_{\alpha\alpha}(\bar{t},t')-\mathbf{g}^>_{\alpha\alpha}(\bar{t},t')\right]\\ &+\int_0^{-i\beta} \mathrm{d}\bar{\tau}\,\mathbf{G}^\rceil_{\mathrm{CC}}(t,\bar{\tau})\mathbf{H}_{\mathrm{C}\alpha}(\bar{\tau})\mathbf{g}^\lceil_{\alpha\alpha}(\bar{\tau},t')\end{aligned} \tag{3.25}$$

and using the definitions of the retarded and advanced Green functions we get

$$\begin{aligned}\mathbf{G}^{<}_{\mathrm{C}\alpha}(t,t') = \int d\bar{t}\Big[&\mathbf{G}^{<}_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{A}_{\alpha\alpha}(\bar{t},t') \\ &+ \mathbf{G}^{R}_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{<}_{\alpha\alpha}(\bar{t},t')\Big] \\ &+ \int_0^{-i\beta} d\bar{\tau}\mathbf{G}^{\rceil}_{\mathrm{CC}}(t,\bar{\tau})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{\lceil}_{\alpha\alpha}(\bar{\tau},t').\end{aligned} \tag{3.26}$$

The current through the lead α then reads

$$\begin{aligned}I_\alpha(t) = -2\mathrm{Re}\Big\{\mathrm{Tr}_{\mathrm{C}}\Big[\int d\bar{t}\big[&\mathbf{G}^{<}_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{A}_{\alpha\alpha}(\bar{t},t') \\ &+ \mathbf{G}^{R}_{\mathrm{CC}}(t,\bar{t})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{<}_{\alpha\alpha}(\bar{t},t')\big]\mathbf{H}_{\alpha\mathrm{C}}(t) \\ &+ \int_0^{-i\beta} d\bar{\tau}\mathbf{G}^{\rceil}_{\mathrm{CC}}(t,\bar{\tau})\mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}^{\lceil}_{\alpha\alpha}(\bar{\tau},t')]\mathbf{H}_{\alpha\mathrm{C}}(t)\Big]\Big\}.\end{aligned} \tag{3.27}$$

This equation can be simplified even further by introducing an embedding self-energy

$$\mathbf{\Sigma}_{\alpha,\mathrm{em}}(t,t') = \mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}_{\alpha\alpha}(t,t')\mathbf{H}_{\alpha\mathrm{C}}, \tag{3.28}$$

which basically describes the effect of leads on the electron states in the central region. Final form for the current reads as follows

$$\begin{aligned}I_\alpha(t) = -2\mathrm{Re}\Big\{\mathrm{Tr}_{\mathrm{C}}\Big[&\int_0^{\infty} d\bar{t}[\mathbf{G}^{<}_{\mathrm{CC}}(t,\bar{t})\mathbf{\Sigma}^{A}_{\alpha,\mathrm{em}}(\bar{t},t) + \mathbf{G}^{R}_{\mathrm{CC}}(t,\bar{t})\mathbf{\Sigma}^{<}_{\alpha,\mathrm{em}}(\bar{t},t)] \\ &+ \int_0^{-i\beta} d\bar{\tau}\mathbf{G}^{\rceil}_{\mathrm{CC}}(t,\bar{\tau})\mathbf{\Sigma}^{\lceil}_{\alpha,\mathrm{em}}(\bar{\tau},t)\Big]\Big\}.\end{aligned} \tag{3.29}$$

The important thing to point out is that this equation depends only known quantities; coupling Hamiltonians and lead Green function via the self-energy term and from the central system Green function $\mathbf{G}_{\mathrm{CC}}$ which is the only unknown we have left. The $\mathbf{G}_{\mathrm{CC}}$ Green function can be solved by finding its equation of motion, which can be found by projecting the Eq. (3.7) to the central region

$$\begin{aligned}[i\partial_t\mathbf{1}_{\mathrm{CC}} - \mathbf{H}_{\mathrm{CC}}(t)]\,\mathbf{G}_{\mathrm{CC}}(t,t') = \delta(t,t')\mathbf{1}_{\mathrm{CC}} &+ \sum_{\alpha=\mathrm{L,R}}\mathbf{H}_{\mathrm{C}\alpha}(t)\mathbf{G}_{\alpha\mathrm{C}}(t,t') \\ &+ \int_\gamma \mathrm{d}\bar{t}\,\mathbf{\Sigma}^{\mathrm{MB}}_{\mathrm{CC}}(t,\bar{t})\mathbf{G}_{\mathrm{CC}}(\bar{t},t')\end{aligned} \tag{3.30}$$

and also to the αC region

$$[i\partial_t\mathbf{1}_{\alpha\alpha} - \mathbf{H}_{\alpha\alpha}(t)]\,\mathbf{G}_{\alpha\mathrm{C}}(t,t') = \mathbf{H}_{\alpha\mathrm{C}}(t)\mathbf{G}_{\mathrm{CC}}(t,t') \tag{3.31}$$

from which it follows that

$$\mathbf{G}_{\alpha\mathrm{C}}(t,t') = \int \mathrm{d}\bar{t}\, \mathbf{g}_{\alpha\alpha}(t,\bar{t})\mathbf{H}_{\alpha\mathrm{C}}(\bar{t})\mathbf{G}_{\mathrm{CC}}(\bar{t},t'). \tag{3.32}$$

Combining the equations (3.30) and (3.32) the equation of motion for the central region Green function $\mathbf{G}_{CC}$ is then found to be

$$\begin{aligned} &\left[i\partial_t \mathbf{1} - \mathbf{H}_{\mathrm{CC}}\right] \mathbf{G}_{\mathrm{CC}}(t,t') \\ &= \delta(t,t')\mathbf{1} + \int_\gamma \mathrm{d}\bar{t}\, \left\{ \left[\mathbf{\Sigma}_{\mathrm{em}}(t,\bar{t}) + \mathbf{\Sigma}^{MB}_{\mathrm{CC}}(t,\bar{t}) \right] \mathbf{G}_{\mathrm{CC}}(\bar{t},t') \right\}, \end{aligned} \tag{3.33}$$

where

$$\mathbf{\Sigma}_{\mathrm{em}}(t,\bar{t}) = \sum_{\alpha=\mathrm{L,R}} \mathbf{\Sigma}_{\alpha,\mathrm{em}}(t,\bar{t}). \tag{3.34}$$

From the equation (3.33) the $\mathbf{G}_{\mathrm{CC}}$ can be solved. The leads arise via the self-energy term $\mathbf{\Sigma}_{\mathrm{em}}$ and therefore only object needed to be changed when changing the form of the leads is the form of this term. The embedding self-energy turns our description from the closed quantum system to the open one.

We have succeeded to write equations describing transport in the open quantum system. The current is expressed in terms of central region Green function and embedding self-energies only. The first two terms in the current-equation (3.29) take the history effects into account while the last term, defined in the imaginary track, describes the initial correlations.

4 Self-energies

In this chapter the different self-energy approximations are studied. The self-energy approximation is required to be Φ-derivable [12, 13] then the observables calculated from the obtained Green function satisfy the conservation laws. Because the different self-energy approximations include different set of Feynman diagrams they also give rise to different history dependencies. At the end of this chapter it is shown how the continuity equation is satisfied if the self-energy is Φ-derivable but at first the form of embedding self-energy for the one-dimensional tight-binding leads is derived.

4.1 Embedding self-energy

The system with discrete states is coupled to the macroscopic leads with continuum of electronic states. This coupling causes the broadening of the central system density of states. The broadening of the states is described by the matrix $\mathbf{\Gamma}$. The effect of the contacts to the central states is accounted by introducing an embedding self-energy matrix $\mathbf{\Sigma}$ which is proportional to the level broadening $\mathbf{\Gamma}$ and to the lead Green function $\mathbf{g}_{\alpha\alpha}$.

The embedding self-energy was defined in the previous chapter as a product of right coupling Hamiltonian, lead Green function and left coupling Hamiltonian as

$$\mathbf{\Sigma}_{\alpha,\mathrm{em}}(t,t') = \mathbf{H}_{\mathrm{C}\alpha}\mathbf{g}(t,t')\mathbf{H}_{\alpha\mathrm{C}}, \tag{4.1}$$

where the matrix elements of the Hamiltonian describe the couplings between the central region and the leads, was found in the last section. The form of these off-diagonal coupling elements of the Hamiltonian were

$$H_{\mathrm{off}} = \sum_{ik}\left[H_{\alpha\mathrm{C},ki}\hat{c}_k^\dagger\hat{c}_i + H_{\mathrm{C}\alpha,ik}\hat{c}_i^\dagger\hat{c}_k\right], \tag{4.2}$$

where the indices i and k label for the basis functions in the central region and leads respectively [11].

The derivation starts by defining the level broadening or level width matrix

$$\Gamma_{ij,\alpha}(\varepsilon) = 2\pi\sum_k V_{i,k\alpha}V_{k\alpha,j}\delta(\varepsilon-\varepsilon_{k\alpha}), \tag{4.3}$$

where we have used a simplifying notation $H_{\mathrm{C}\alpha,ik} \equiv V_{i,k\alpha}$ and $H_{\alpha\mathrm{C},ki} \equiv V_{k\alpha,i} \equiv V^*_{k\alpha,i}$. From this equation it is seen that, more strongly the system is coupled to leads more broaden states will be. The self-energy can be rewritten with help of the greater and lesser component of the lead Green function and level broadening Γ. This gives us an expression for the embedding self-energy in which the only unknown parameter is the level broadening.

4.1.1 The lead Green function

If the indices k and l label non-local one particle eigenstates (eigenenergies $\varepsilon_{\alpha k}$) in the leads the lead Green function $\mathbf{g}_{\alpha\alpha}$ in the molecular basis where the Hamiltonian is diagonal can be solved as follows. Starting from the definition of the lesser lead Green function [11, 14]

$$\mathbf{g}^{<}_{\alpha\alpha,kl}(t,t') = i\langle \hat{c}^\dagger_{\alpha l}(t')\hat{c}_{\alpha k}(t)\rangle = i\hat{S}_{li}(t')\langle \hat{c}^\dagger_{\alpha i}(0)\hat{c}_{\alpha j}(0)\rangle \hat{S}^\dagger_{jk}(t), \tag{4.4}$$

where $\hat{S}(t)$ is the one-electron evolution matrix and the time-evolution of a operator $\hat{c}$ is given by

$$\hat{c}_k(t) = \sum_n \hat{S}_{kl}\hat{c}_l(0), \tag{4.5}$$

$$\hat{c}^\dagger_k(t) = \sum_n \hat{c}^\dagger_l(0)\hat{S}^\dagger_{lk}. \tag{4.6}$$

The evolution operator $\hat{S}$ satisfies following equation of motion (with boundary condition $\hat{\mathbf{S}}(0) = 1$)

$$i\partial_t \hat{\mathbf{S}}(t) = \hat{\mathbf{h}}(t)\hat{\mathbf{S}}(t), \tag{4.7}$$

where $\hat{h}$ is given by a general Hamiltonian $H(t) = \sum_{ij} h_{ij}(t)\hat{c}^\dagger_i\hat{c}_j$. For diagonal Hamiltonian of the form $\hat{H}_{lead}(t) = \sum_{k\alpha}[\varepsilon_{k\alpha} + U_\alpha(t)]\hat{c}^\dagger_{k\alpha}\hat{c}_{k\alpha}$ this equation can be solved to obtain

$$\hat{S}^\alpha_{kl} = \delta_{kl}e^{-i\int_0^t \mathrm{d}t'\,[\varepsilon_{k\alpha}+U_\alpha(t')]}, \tag{4.8}$$

where in the last step the cyclic property of the trace is used to rewrite the numerator as

$$\langle \hat{c}^\dagger_{\alpha i}(0)\hat{c}_{\alpha j}(0)\rangle = \frac{\mathrm{Tr}\left\{e^{-\beta H}\hat{c}^\dagger_{\alpha i}(0)\hat{c}_{\alpha j}(0)\right\}}{\mathrm{Tr}\left\{e^{-\beta H}\right\}} = \frac{\mathrm{Tr}\left\{\hat{c}_{\alpha j}(0)e^{-\beta H}\hat{c}^\dagger_{\alpha i}(0)\right\}}{\mathrm{Tr}\left\{e^{-\beta H}\right\}}. \tag{4.9}$$

Recalling that in the Heisenberg picture where the operators are time-dependent the operator $\hat{O}(t)$ has expression $\hat{O}(t) = e^{\beta H}\hat{O}e^{-\beta H}$. Therefore, writing the operator $\hat{c}_{l\alpha}(t)$ as $\hat{c}_{l\alpha}(t) = e^{\beta H}\hat{c}_{l\alpha}(0)e^{-\beta H}$ and taking a time derivative with respect to β we get [14]

$$e^{\beta H}\hat{c}_{j\alpha}(0)e^{-\beta H} = \sum_{i\alpha}\left(e^{-\beta \mathbf{h}}\right)_{ij} e^{\beta H}\hat{c}_{i\alpha}(0)e^{-\beta H}. \tag{4.10}$$

This equation has a solution

$$\mathbf{a}(\beta) = e^{-\beta \mathbf{h}} \mathbf{a}(0). \tag{4.11}$$

Multiplying from left with $e^{-\beta H}$ we end up to following equation

$$c_j(0) e^{-\beta H} = \sum_i \left(e^{-\beta H} \right)_{ij} e^{-\beta H} \hat{c}_i. \tag{4.12}$$

Inserting this expression for $c_j(0)e^{-\beta H}$ to the equation (4.9) and after some algebra the expectation value of a product of creation and annihilation operators is found to be the generalized Fermi-distribution

$$\begin{aligned} \langle \hat{c}^\dagger_{\alpha i}(0) \hat{c}_{\alpha j}(0) \rangle &= \frac{\mathrm{Tr}\left\{ \hat{c}_{\alpha j}(0) e^{-\beta H} \hat{c}^\dagger_{\alpha i}(0) \right\}}{\mathrm{Tr}\left\{ e^{-\beta H} \right\}} \\ &= \sum_i \left[\left(e^{-\beta \mathbf{h}} \right)_{ij} \frac{\mathrm{Tr}\left\{ e^{-\beta H} \delta_{ij} \right\}}{\mathrm{Tr}\left\{ e^{-\beta H} \right\}} - \left(e^{-\beta \mathbf{h}} \right)_{ij} \frac{\mathrm{Tr}\left\{ e^{-\beta H} \hat{c}^\dagger_{\alpha i} \hat{c}_{\alpha j} \right\}}{\mathrm{Tr}\left\{ e^{-\beta H} \right\}} \right] \\ &= \left(\frac{1}{e^{\beta H} + 1} \right)_{ij} = \frac{\delta_{ij}}{e^{\beta \varepsilon_i} + 1} = f(\varepsilon_i), \end{aligned} \tag{4.13}$$

where we have assumed that the Hamiltonian is diagonal. Thus, the greater and lesser components of lead Green functions are

$$g^<_{\alpha\alpha,kl}(t,t') = i\delta_{kl} f(\varepsilon_{k\alpha}) e^{-i\int_{t'}^{t} \mathrm{d}\bar{t}\,[\varepsilon_{k\alpha} - U_\alpha(\bar{t})]}, \tag{4.14}$$

$$g^>_{\alpha\alpha,kl}(t,t') = i\delta_{kl} [f(\varepsilon_{k\alpha}) - 1] e^{-i\int_{t'}^{t} \mathrm{d}\bar{t}\,[\varepsilon_{k\alpha} - U_\alpha(\bar{t})]}. \tag{4.15}$$

4.1.2 One dimensional tight-binding leads

To derive an explicit expression for the embedding self-energy, the leads are treated using tight-binding approximation. The tight-binding Hamiltonian has the form

$$\hat{H} = \sum_{ij} t_{ij} \hat{c}^\dagger_i \hat{c}_j, \tag{4.16}$$

where the creation and annihilation operators $\hat{c}^\dagger_i,\ \hat{c}_j$ are defined in the localized site basis. Diagonal elements $t_{ii} = a$ describe the orbital energy, or the on-site energy, of the site i, which describes the energy of placing an electron to a site i. The t_{ij} term ($i, j \in \{nearest\ neighbors\}$) is the hopping term, which describe the possibility for electrons to hop from site to the next and produces an "interaction" energy between electrons located at different sites [11].

Because the tight-binding Hamiltonian describes the system in the localized basis and the lead Green function is defined in the non-local basis we need a basis transformation

between these two basis representations. Let the $\hat{\psi}(x)$ be the field operator in the localized basis and $\hat{\chi}$ the field operator in the non-local molecular orbital basis. The transformation between these two different bases is given by the transformation matrix $\mathbf{D}$, which diagonalizes the Hamiltonian $D^\dagger H D = \mathrm{diag}[\varepsilon_k]$

$$\hat{\chi}_j(x) = \sum_k D_{kj}\hat{\phi}_k(x). \tag{4.17}$$

In this basis transform the ij-component of the lead Green function transforms as

$$g_{ij}(t,t') = \left[D\tilde{g}(t,t')D^\dagger\right]_{ij}. \tag{4.18}$$

Therefore, the greater and lesser components are

$$g^{>}_{ij}(t,t') = i\sum_k D_{ik}[f(\varepsilon_{k\alpha})-1]e^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,(\varepsilon_{k\alpha}-U_\alpha(\bar{t}))}D^\dagger_{kj} \tag{4.19}$$

$$g^{<}_{ij}(t,t') = i\sum_k D_{ik}f(\varepsilon_{k\alpha})e^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,(\varepsilon_{k\alpha}-U_\alpha(\bar{t}))}D^\dagger_{kj} \tag{4.20}$$

For example, the greater component of the embedding self-energy is now

$$\begin{aligned}\Sigma^{<}_{ij,\alpha,\mathrm{em}}(t,t') &= \sum_{kl} V_{i,k\alpha}g^{<}_{kl}(t,t')V_{l\alpha,j}\\ &= i\sum_{kl}\sum_m V_{i,k\alpha}D_{km}f(\varepsilon_{m\alpha})e^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,(\varepsilon_{k\alpha}-U_\alpha(\bar{t}))}D^\dagger_{ml}V_{l\alpha,j}\\ &= ie^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,U_\alpha(\bar{t})}\int\frac{d\varepsilon}{2\pi}f(\varepsilon)\Gamma_{ij,\alpha}(\varepsilon)e^{-i\varepsilon(t-t')},\end{aligned} \tag{4.21}$$

where the transformed level broadening is used

$$\Gamma_{ij,\alpha}(\varepsilon) = 2\pi\sum_{klm} V_{i,k\alpha}D_{km}\delta(\varepsilon-\varepsilon_{m\alpha})D^\dagger_{ml}V_{l\alpha,j}. \tag{4.22}$$

In general this allows us to write lesser and greater component for embedding self-energy as follows

$$\begin{aligned}\Sigma^{<}_{ij,\alpha,\mathrm{em}}(t,t') &= \sum_{kl} V_{i,k\alpha}g^{<}_{kl}(t,t')V_{l\alpha,j}\\ &= \frac{i}{2\pi}e^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,U_\alpha(\bar{t})}\int\mathrm{d}\varepsilon\,\Gamma_{ij,\alpha}(\varepsilon)f(\varepsilon)e^{-i\varepsilon(t-t')},\end{aligned} \tag{4.23}$$

$$\begin{aligned}\Sigma^{>}_{ij,\alpha,\mathrm{em}}(t,t') &= \sum_{kl} V_{i,k\alpha}g^{>}_{kl}(t,t')V_{l\alpha,j}\\ &= \frac{i}{2\pi}e^{-i\int_{t'}^{t}\mathrm{d}\bar{t}\,U_\alpha(\bar{t})}\int\mathrm{d}\varepsilon\,\Gamma_{ij,\alpha}(\varepsilon)[f(\varepsilon)-1]e^{-i\varepsilon(t-t')}.\end{aligned} \tag{4.24}$$

Only the first sites from the lead are coupled to the sites in the central system. As a results the coupling terms $V_{i,k\alpha}$ and $V_{l\alpha,j}$ can have a nonzero elements when t he lead index is 1. This allows us to write

$$V_{i,k\alpha} = \delta_{k,1} V_{i,k\alpha}, \tag{4.25}$$
$$V_{l\alpha,j} = = \delta_{l,1} V_{l\alpha,j}. \tag{4.26}$$

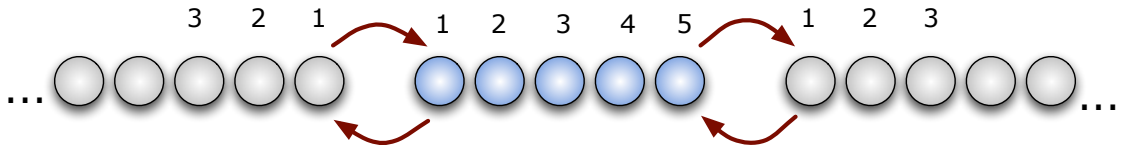

Figure 4.1: Schematic picture of the system. Only the first lead sites are coupled with the sites of the central system.

The level-broadening matrix can now be written as

$$\Gamma_{ij,\alpha}(\varepsilon) = 2\pi V_{i,1} V_{1,j} \sum_{m=1}^{l} D_{1m} \delta(\varepsilon - \varepsilon_{m\alpha}) D^{\dagger}_{m1} \tag{4.27}$$

Determination of the explicit form of the broadening matrix $\mathbf{\Gamma}$ requires determining the eigenvalues of the tight-binding Hamiltonian. The eigenvalues can be solved from the determinant

$$\mathrm{Det}(H - I\lambda) = \begin{vmatrix} a-\lambda & b & 0 & 0 & \dots \\ b & a-\lambda & b & 0 & \\ 0 & b & a-\lambda & 0 & \\ 0 & 0 & b & a-\lambda & \\ \vdots & & & & \ddots \\ & & & & \end{vmatrix}. \tag{4.28}$$

The sub-determinants satisfy the following recurrence equation [11]

$$D_{l+2} = cD_{l+1} - b^2 D_l, \tag{4.29}$$
$$D_2 = c^2 - b^2, \tag{4.30}$$
$$D_1 = c. \tag{4.31}$$

The eigenvalues or the eigenenergies of the tight-binging lead are then

$$\lambda_k = a \pm 2b \cos\left(\frac{\pi k}{l+1}\right). \tag{4.32}$$

The eigenvectors obey the equation $(H - I\lambda_k)x^{(k)} = 0$, which leads to a recurrence equation for vector components $x_n^{(k)}$, $n = 1, ..., l-1$ [11],

$$bx_{n+2}^{(k)} + cx_{n+1}^{(k)} + bx_n^{(k)} = 0 \tag{4.33}$$

with boundary conditions

$$x_1^{(k)} = 1 \tag{4.34}$$

$$x_2^{(k)} = -c/b = -2\cos(\phi_k),\ \phi_k = (2\pi)/(l+1),\ k = 1, ...l \tag{4.35}$$

$$x_n^{(k)} = 0,\ n \leq 0 \ \text{ or } \ n > l. \tag{4.36}$$

The eigenvectors are then

$$x_n^{(k)} = (-1)^{n+1}\sqrt{\frac{2}{l+1}}\sin\left(\frac{n\pi k}{l+1}\right), \tag{4.37}$$

where $k = 1, ..., l$ and $n = 1, ..., l$. The level-broadening matrix can now be written with these eigenvectors as

$$\Gamma_{ij,\alpha}(\varepsilon) = 2\pi V_{i,1}V_{1,j}\sum_{m=1}^{l} x_1^{(m)}\delta(\varepsilon - \varepsilon_{m\alpha})x_1^{(m)}. \tag{4.38}$$

The summation over m can be turned into a integration by assuming a macroscopic leads which implies that $l \to \infty$.

$$\Gamma_{ij,kl,\alpha}(\varepsilon) = 2\pi V_{i,k\alpha}V_{l\alpha,j}\frac{2}{l+1}\int_q^l dm\sin^2(\frac{\pi m}{l+1})\delta(\varepsilon - \varepsilon_{m\alpha}), \tag{4.39}$$

where $\varepsilon_{m\alpha} = a + 2b\cos(\frac{m\pi}{l+1}) - \mu$. Changing the integration variables according to $y = -2b\cos\left(\frac{m\pi}{l+1}\right) \Rightarrow \cos\left(\frac{m\pi}{l+1}\right) = -\frac{-y}{2b}$ and using an identity $\sin^2\left(\frac{m\pi}{l+1}\right) = 1 - \frac{y^2}{4b^2}$ gives an expression for the level broadening

$$\begin{aligned}\Gamma_{ij,\alpha}(\varepsilon) &= \frac{2V_{i,1}V_{1,j}}{b}\int_{-2b}^{2b} dy\sqrt{1 - \frac{y^2}{4b^2}}\delta(\varepsilon - a + \mu - y) \\ &= \frac{2V_{i,1}V_{1,j}}{b}\sqrt{1 - \frac{\tilde{\varepsilon}^2}{4b^2}}\theta(2b - |\tilde{\varepsilon}|).\end{aligned} \tag{4.40}$$

Inserting this equation to the equations of the greater and lesser components of the embedding self-energies we obtain following equations defined on the real axis:

$$\begin{aligned}\Sigma_{ij,\alpha,\mathrm{em}}^{<}(t,t') = i\frac{V_{i,1}V_{1,j}}{b\pi}e^{-i\int_{t'}^{t}\,\mathrm{d}\bar{t}U_\alpha(\bar{t})}\int_{a-2b}^{a+2b}\mathrm{d}\varepsilon\, f(\varepsilon - \mu) \\ \times\sqrt{1 - \frac{\varepsilon^2}{4b^2}}e^{-i(\varepsilon-\mu)(t-t')},\end{aligned} \tag{4.41}$$

$$\begin{aligned}\Sigma_{ij,\alpha,\mathrm{em}}^{>}(t,t') = i\frac{V_{i,1}V_{1,j}}{b\pi}e^{-i\int_{t'}^{t}\,\mathrm{d}\bar{t}U_\alpha(\bar{t})}\int_{a-2b}^{a+2b}\mathrm{d}\varepsilon\,[f(\varepsilon - \mu) - 1] \\ \times\sqrt{1 - \frac{\varepsilon^2}{4b^2}}e^{-i(\varepsilon-\mu)(t-t')}.\end{aligned} \tag{4.42}$$

The other components needed to propagate the Kadanoff-Baym equations can be obtained from these expressions since

$$\begin{aligned}
\mathbf{\Sigma}^{\rceil}(\mathbf{x}t, \mathbf{x}'\tau') &= \mathbf{\Sigma}^{<}(\mathbf{x}t, \mathbf{x}'t_0 - i\tau'), && (4.43)\\
\mathbf{\Sigma}^{\lceil}(\mathbf{x}\tau, \mathbf{x}'t') &= \mathbf{\Sigma}^{>}(\mathbf{x}t_0 - i\tau, \mathbf{x}'t'), && (4.44)\\
\mathbf{\Sigma}^{M}(\mathbf{x}\tau, \mathbf{x}'\tau') &= \mathbf{\Sigma}(\mathbf{x}t_0 - i\tau, \mathbf{x}'t_0 - i\tau'). && (4.45)
\end{aligned}$$

Matsubara component defined purely on the imaginary axis:

$$\begin{aligned}
\Sigma^{M}_{ij,\alpha,\mathrm{em}}(-i\tau_1, -i\tau') = i\frac{V_{i,1}V_{1,j}}{b\pi}\int_{a-2b}^{a+2b} \mathrm{d}\varepsilon\, f(\varepsilon-\mu) \\
\times\sqrt{1-\frac{\varepsilon^2}{4b^2}}e^{-(\varepsilon-\mu)(\tau-\tau')}. \qquad (4.46)
\end{aligned}$$

(4.47)

The mixed components, having both imaginary and real time-arguments:

$$\begin{aligned}
\Sigma^{\lceil}_{ij,\alpha,\mathrm{em}}(t, -i\tau') = i\frac{V_{i,1}V_{1,j}}{b\pi}e^{-i\int_0^{t'}\mathrm{d}\bar{t}U_\alpha(\bar{t})}\int_{a-2b}^{a+2b} \mathrm{d}\varepsilon\, f(\varepsilon-\mu) \\
\times\sqrt{1-\frac{\varepsilon^2}{4b^2}}e^{-i(\varepsilon-\mu)(t+i\tau')}, \qquad (4.48)\\
\Sigma^{\rceil}_{ij,\alpha,\mathrm{em}}(-i\tau, t') = i\frac{V_{i,1}V_{1,j}}{b\pi}e^{-i\int_t^{0}\mathrm{d}\bar{t}U_\alpha(\bar{t})}\int_{a-2b}^{a+2b} \mathrm{d}\varepsilon\, [f(\varepsilon-\mu)-1] \\
\times\sqrt{1-\frac{\varepsilon^2}{4b^2}}e^{-i(\varepsilon-\mu)(-i\tau-t')}. \qquad (4.49)
\end{aligned}$$

We have now derived the equation for current and for the embedding self-energy. What is missing is the many-body self-energy and this will be the concept of following section.

4.2 Many-body self-energy approximations

Solving the equation of motion for the Green function seems to be a rather complicated task due to the appearance of the higher order Green functions. Two different ways to tackle this problem are to approximate the two-particle Green function in terms of collisions (collision approximation) or introduce the function Σ to formally solve the integro-differential equation and to get a solution of the form

$$[i\partial_{t_1} - \hat{h}(1)]G(1,2) = \delta(1,2) + \int \mathrm{d}3\, \Sigma(1,3)G(3,2) \tag{4.50}$$

$$[-i\partial_{t_2} - \hat{h}(2)]G(1,2) = \delta(1,2) + \int \mathrm{d}3\, G(1,3)\hat{\Sigma}(3,2), \tag{4.51}$$

where $\hat{\Sigma}$ is the adjoint of the self-energy operator Σ and for systems initially in the equilibrium these self-energies are the same, *i.e.*, $\hat{\Sigma} = \Sigma$.

This trick of solving the equation of motion is mathematically justified and used as a tool to solve problems of this from. The self-energy operator includes all of the interaction effects of the particle within itself. Comparing the Fourier-transforms of the noninteracting Green function to the interacting one it is seen that the effect of the self-energy is to shift the poles of the Green function compared to the noninteracting Green function. Therefore, the self-energy can be considered as a contribution to the energy of the excitations of the system from the interaction effects.

In the chapter 2 we considered the expectation values of the operators and observed them to be proportional to the single-particle Green function $G(1,2)$. Therefore the expectation values depend on the approximation scheme used to obtain the Green function. The requirement for the approximations is, hence, that they satisfy the macroscopic conservation laws. In the transport problems it is natural to require the validity of the continuity equation $\partial_t\langle\hat{n}\rangle = -\nabla\cdot\langle\mathbf{j}\rangle$. In the next sections we look at three different conserving self-energy approximations: Hartree-Fock, second Born and GW-approximations. The Hartree-Fock and second Born approximations are interpreted also approximating directly the two-particle Green function.

4.2.1 Hartree-Fock approximation

The Hartree-Fock approximation is a lowest order approximation for the many-body effects. In this approximation the interactions among the electrons are neglected leading to a treatment of the electrons as noninteracting quasi-particles. Hartree approximation tells us that, after adding particles to the system they will be propagating independently of each other and independently of the other particles. This gives us

an approximation for the two-particle Green function as a product of the two single-particle Green functions

$$G(1,3;3^+,2) = G(1,2)G(3,3^+). \tag{4.52}$$

Plugging this into the equation of motion

$$\left[i\partial_{t_1} - \hat{h}(1)\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\, w(1,3)G(1,3;3^+,2) \tag{4.53}$$

gives us the Hartree approximation

$$\left[i\partial_t - \hat{h}(1) - \int \mathrm{d}3\, w(1,3)\langle\hat{n}(3)\rangle\right] G(1,2) = \delta(1,2), \tag{4.54}$$

where the $\int d3w(1,3)\langle\hat{n}(3)\rangle$ term represents self-consistent potential field generated by all the other particles.

The drawback of Hartree approximation is that it does not include the indistinguishableness of the electrons. The two processes where particle starting at state 1 appears at 2 form the process where it appears at 3^+. This can be taken into account by adding one extra term to our two-particle Green function approximation

$$G(1,3;3^+,2) = G(1,2)G(3,3^+) \pm G(1,3^+)G(3,2). \tag{4.55}$$

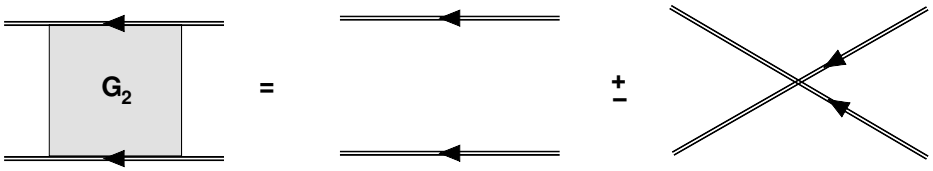

Figure 4.2: Hartree-Fock approximation for the two-particle Green function

Inserting this approximation to the equation of motion gives

$$\left[i\partial_{t_1} - \hat{h}(1) + \int \mathrm{d}3\, w(1,3)\langle\hat{n}\rangle\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\, w(1,3)G(1,3^+)G(3,2), \tag{4.56}$$

where the term $\int \mathrm{d}3\, w(1,3)\langle\hat{n}\rangle$ is the Hartree term, which describes the interaction with the uniform background charge induced by all the other particles. The second term $\int \mathrm{d}3\, w(1,3)G(1,3^+)G(3,2)$ is the Fock-term, which takes into account the exchange interaction.

Assuming translationally invariant system it is possible to found an expression for the spectral function within Hartree-Fock approximation. Performing the Fourier-transform for the equation of motion we get

$$[\omega - \varepsilon_{HF}(\omega)]\, G(\omega) = 1, \tag{4.57}$$

where $\varepsilon_{HF}(\omega) = \varepsilon + nv \pm \int \frac{d\omega'}{(2\pi)^3} v(\omega - \omega')\langle \hat{n}(\omega')\rangle$ is the Fourier-transform of kinetic energy and the Hartree-Fock potential. The Fourier-transform of the Green function is therefore

$$G(\omega) = \frac{1}{\omega - \varepsilon_{HF}(\omega)}. \tag{4.58}$$

Spectral function, being proportional to the imaginary part of the retarded Green function, is now proportional to the delta function $A(\omega) \propto \delta(\omega - \varepsilon_{HF}(\omega))$. Thus, the quasiparticle states appear to be discrete set of energy states with no lifetime. In the Hartree-Fock approximation there is no possibility for collisions between the particles and therefore no mechanism, which could cause the change of the state of the particle and redistribute the energies.

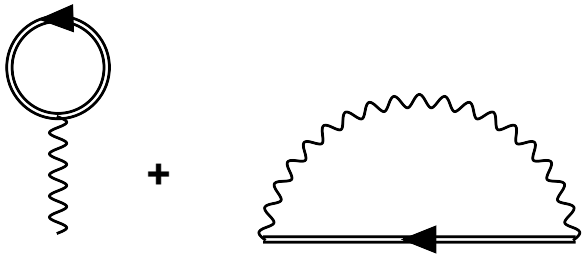

Figure 4.3: Hartree-Fock self-energy (Feynman) diagrams.

4.2.2 Second Born approximation

To obtain finite lifetime for the quasi-particle states we have to improve our approximation scheme and include scattering mechanisms. A simplest type of scattering process is that when particles propagating from points 1 and 3 to points 2 and 3^+ the potential acts at point 4 between the particles and scatters them. The corresponding approximation for the two-particle Green function reads

$$G(1,3;3^+,2) = G(1,2)G(3,3^+) \pm G(1,3^+)G(3,2)$$
$$+ \int \mathrm{d4d5}\; w(4,5)\left[G(1,4)G(4,2)G(3,5)G(5,3^+) \pm G(1,4)G(4,2)G(3,5)G(5,2)\right]. \tag{4.59}$$

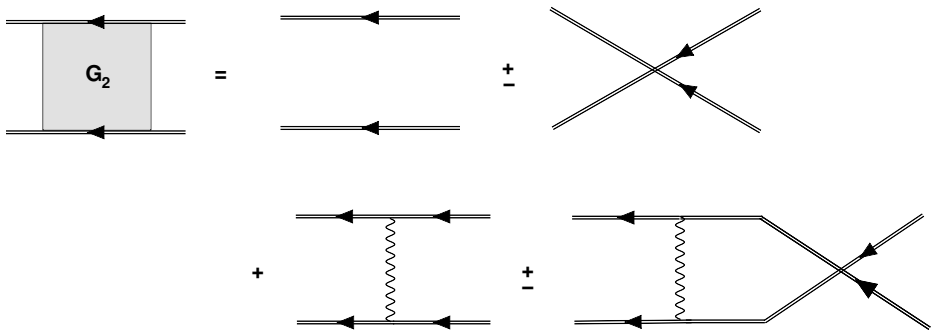

Figure 4.4: Second Born approximation for the two-particle Green function

This procedure could be, in principle, continued to obtain higher order corrections, but it is getting ugly. But all in all, introducing the self-energy Σ and trying to find approximations for it, is a more efficient and cleaner way to solve the equation of motion of the Green function. It is needed to be noted that, the approximation for self-energy Σ cannot be chosen freely since it has to be obtained from some approximate Φ-functional according to

$$\Sigma(1,2) = \frac{\delta\Phi[G]}{\delta G(2,1)}, \tag{4.60}$$

then the calculated observables satisfy the macroscopic conservation laws, like continuity equation. This was proven by Baym at 1962 [12].

Our next task is to solve the equation of motion self-consistently. Our starting point is the definition of the time-evolution operator on the contour γ as

$$\hat{U}(t,t') = \mathcal{T}_{\mathcal{C}}\left[\exp\left(-i\int d\tilde{t}\hat{H}(\tilde{t})\right)\right]. \tag{4.61}$$

Making small variations to the Hamiltonian causes a change in $\hat{U}$ and these changes can be investigated by using the previous exponential expression as a generating functional. A small perturbation $\delta\hat{V}(t)$ to the Hamiltonian, causes a following change $\delta\hat{U}(t,t')$ to the time-evolution operator (see Appendix E)

$$\delta\hat{U}(t,t') = -i\int_{t'}^{t} \mathrm{d}\tau\ \hat{U}(t,\tau)\delta\hat{V}(\tau)\hat{U}(\tau,t'). \tag{4.62}$$

If the external perturbation is taken to be of the form $\delta\hat{V} = \int \mathrm{d}\mathbf{x}\,\delta v(\mathbf{x}t)\hat{n}(\mathbf{x})$, where $\hat{n}(\mathbf{x}) = \hat{\psi}^{\dagger}(x\mathbf{x})\hat{\psi}(\mathbf{x})$ is the density operator. Then the change in $\hat{U}$ due to external perturbation $V(\mathbf{x}t)$ is

$$\frac{\delta\hat{U}(t,t')}{\delta v(\mathbf{x}t)} = i\hat{U}(t_0 - i\beta, t_0)\hat{n}_H(\mathbf{x}t). \tag{4.63}$$

Using this equation we can calculate the change in expectation values due to v, and especially the change in the expectation value of the time-ordered product of two operators $\delta\langle\mathcal{T}_\mathcal{C}\left[\hat{A}(t_1)\hat{B}(t_2)\right]\rangle/\delta v(3)$ (see Appendix E). The functional derivative of the Green function with respect to the external perturbation can readily found to be

$$\begin{aligned}\frac{\delta G(1,2)}{\delta v(3)} &= -i\frac{\delta}{\delta v(3)}\langle\mathcal{T}_\mathcal{C}[\hat{\psi}(1)\hat{\psi}^\dagger(2)]\rangle \\ &= \langle\mathcal{T}_\mathcal{C}[\hat{\psi}(1)\hat{\psi}^\dagger(2)\hat{n}_H(3)]\rangle + \langle\hat{n}_H(3)\rangle\langle\mathcal{T}_\mathcal{C}[\hat{\psi}(1)\hat{\psi}^\dagger(2)]\rangle,\end{aligned} \tag{4.64}$$

from which it follows that

$$\langle\mathcal{T}_\mathcal{C}[\hat{\psi}^\dagger(3)\hat{\psi}(3)\hat{\psi}(1)\hat{\psi}^\dagger(2)]\rangle = i\frac{\delta G(1,2)}{\delta v(3)} + \langle n_H(3)\rangle G(1,2). \tag{4.65}$$

Substituting this into the equation of motion gives

$$\begin{aligned}\left[i\partial_{t_1} - \hat{h}(1)\right]G(1,2) = \delta(1,2) + i\int \mathrm{d}3\, w(1,3)\frac{\delta G(1,2)}{\delta v(3)} \\ + G(1,2)\int \mathrm{d}3\; w(2^+,3)\langle\hat{n}_H(3)\rangle.\end{aligned} \tag{4.66}$$

From the definition of the inverse Green function $\int G(1,2)G^{-1}(2,1) = \delta(1,2)$ the functional derivative of the Green function with respect to the external potential $v(3)$ can be derived

$$\begin{aligned}\frac{\delta G(1,2)}{v(3)} &= -\int \mathrm{d}4\mathrm{d}5\, G(1,4)\frac{\delta G^{-1}(4,5)}{\delta v(3)}G(5,2) \\ &= \int \mathrm{d}4\mathrm{d}5\, G(1,4)\Gamma(45;3)G(5,2),\end{aligned} \tag{4.67}$$

where we have defined the vertex function $\Gamma(45;3)$ as

$$\Gamma(45;3) = -\frac{\delta G^{-1}(4,5)}{\delta v(3)}. \tag{4.68}$$

Because $G^{-1}(1,2) = [\partial_{t_1} - \hat{h}(1)]\delta(1,4) - \Sigma(1,4)$ the vertex function can be also written as

$$\Gamma(1,4;3) = \delta(1,3)\delta(1,4) + \frac{\delta\Sigma(1,4)}{\delta v(3)}. \tag{4.69}$$

Inserting the equation (4.67) to the equation of motion we have an equation where the self-energy term can be picked

$$\begin{aligned}&[i\partial_{t_1} - h(1)]\,G(1,1') \\ &= \delta(1,1') + \int \mathrm{d}4\left[i\int \mathrm{d}2\mathrm{d}3\; G(1,3)w(1,2)\Gamma(3,4;2)\right. \\ &\left. + \delta(1,4)\delta(3,2)w(4,3)\langle\hat{n}_H(3)\rangle\right]G(4,1').\end{aligned} \tag{4.70}$$

Therefore we can write the self-energy Σ as

$$\Sigma(1,4) = i \int \mathrm{d}2\mathrm{d}3 \left[G(1,3)w(1,2)\Gamma(3,4;2) + \delta(1,2)w(1,3)G(3,3^+) \right]. \tag{4.71}$$

From this expression it is possible to generate higher order self-energy approximations iteratively by inserting the definition of the vertex function

$$\begin{aligned} \Sigma(1,2) = iG(1,2)w(1^+,2) + i\delta(1,2) \int \mathrm{d}3\, w(1,3)G(3,3^+) \\ +i \int \mathrm{d}4\mathrm{d}5\; G(1,3)w(1^+,4)\frac{\delta\Sigma(3,2)}{\delta v(4)}. \end{aligned} \tag{4.72}$$

Using the first-order approximation for the vertex function $\Gamma(12;3) = \delta(1,2)\delta(1,3)$ gives the first-order approximation for the self-energy namely the Hartree-Fock approximation

$$\Sigma(1,2) = iG(1,2)w(1^+,2) + i\delta(1,2) \int \mathrm{d}3\, w(1,3)G(3,3^+). \tag{4.73}$$

If we make a first iteration for the equation (4.71) we obtain the Second Born approximation for the electron self-energy

$$\begin{aligned} \Sigma^{2B}(1,2) = \Sigma^{HF}(1,2) + i^2 \int \mathrm{d}3\mathrm{d}4\, G(1,3)w(1^+,4)G(3.4)G(4,2)w(3^+,2) \\ -i^2 \int \mathrm{d}4\mathrm{d}5\; G(1,2)w(1^+,4)w(2,5)G(5,4)G(4,5^+), \end{aligned} \tag{4.74}$$

where in addition to the time-local part of the self-energy (Σ^{HF}) we have terms second order in w. Thus the second Born approximation includes Hartree-Fock approximation added the first-order polarization insertion and the second order approximation for the exchange correction.

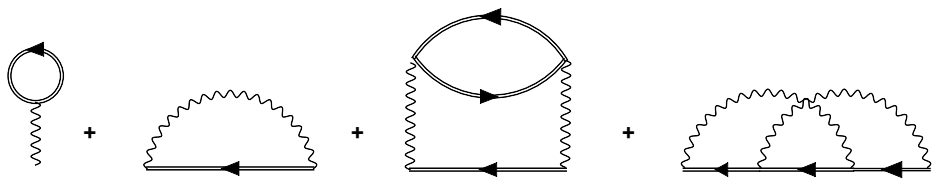

Figure 4.5: Second Born approximation self-energy (Feynman) diagrams.

The addition of these extra corrections to the self-energy causes the many-electron system described by the delta-function energy levels towards system with finite lifetime of the states. This can be seen for example by looking the Fourier-transform of the Green function, which can be written as follows

$$G(\omega) = \frac{1}{\omega - \varepsilon - \Sigma} = \frac{1}{\omega - \varepsilon - \mathrm{Re}(\Sigma) + i\mathrm{Im}(\Sigma)}. \tag{4.75}$$

The real part of the self-energy causes a shift of the energy levels of the system while the imaginary part gives the eigenstates a finite lifetime. The spectral function being proportional to the imaginary part of the retarded Green function is

$$A(\omega) \propto \frac{\mathrm{Im}(\Sigma)}{(\omega - \varepsilon - \mathrm{Re}\Sigma)^2 + (\mathrm{Im}(\Sigma))^2}, \tag{4.76}$$

which is a Lorentzian-form. The height of the peak is proportional to $1/\mathrm{Im}(\Sigma)$ and the half-width at half-maximum is specified by $\mathrm{Im}\Sigma$.

4.2.3 GW approximation

In real systems the long-range interactions can be more significant compared to the short-range interactions, the later taken into account by the second Born approximation. In this chapter the basic idea behind the GW approximation, which includes a description of the long range and screening effects, is presented. The GW approximation can be considered as a generalization of Hartree-Fock approximation with dynamically screened Coulomb interaction.

The derivation of the GW equations starts the same way as for the second Born approximation. We have the equation of motion for Green function with time-ordered product of four field operators

$$\left[i\partial_{t_1} - \hat{h}(1)\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\; w(1,3)\mathcal{T}_{\mathcal{C}}[\hat{\psi}^\dagger(3)\hat{\psi}(3)\hat{\psi}(1)\hat{\psi}^\dagger(2)]. \tag{4.77}$$

In the last section we found that the time-ordered product of four field operators is equal to the functional derivative of the one-particle Green function with respect to the external perturbation plus the product of expectation value of the density operator and the one-particle Green function. To derive this equation we needed to find what is the change in the time-evolution operator due to a small change in the Hamiltonian. Using the equation (4.64) we obtain a following form for the Green function EOM

$$\left[i\partial_{t_1} - \hat{h}(1) - V(1)\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\; w(1,3)\frac{\delta G(1,2)}{\delta v(3)}, \tag{4.78}$$

where

$$V(1) = v(1) + \int \text{d3}\; w(1,3)\langle \hat{n}_H(3)\rangle. \tag{4.79}$$

Comparing this equation with the equation

$$[i\partial_{t_1} - \hat{h}(1)]G(1,2) = \delta(1,2) + \int \text{d3}\; \Sigma(1,3)G(3,2) \tag{4.80}$$

and using the definition of the vertex function, the self-energy can be expressed as follows

$$\Sigma(1,2) = -i \int \text{d3d4}\; w(1,3^+)G(1,4)\frac{\delta G^{-1}(4,2)}{v(3)}. \tag{4.81}$$

Changes in the potential δV are consequences of the changes in the external potential δv plus changes in the particle density, *i.e.*,

$$\delta V(1) = \delta v(1) + \int \text{d3}\; w(1,3)\langle \delta n(3)\rangle. \tag{4.82}$$

This equation tells us that the change in the total single particle potential is important not the changes in the external potential. Including the effective interaction of the electrons we define the screened coulomb interaction as

$$W(1,2) = \int \text{d3}\; w(1,3)\frac{\delta V(2)}{\delta v(3)}. \tag{4.83}$$

This describes the effect of test charge at point 2, including the polarization effects to the potential at point 1. The form of this equation can be justified by thinking a classical analogy where the screening is defined in terms of dielectric constant ϵ as $V_{ind} = v_{exl}/\epsilon$. Now the dielectric response is defined as

$$\epsilon^{-1}(1,2) = \frac{\delta V(1)}{\delta v(2)}. \tag{4.84}$$

Using previous definitions and earlier derived equations one can readily convince herself/himself that this screened interaction can be expressed as

$$W(1,2) = w(1,2) + i \int \text{d3d4}\; W(1,3)P(3,4)w(4,2), \tag{4.85}$$

where we have defined the polarization propagator as

$$P(1,3) = \int \text{d4d5}\; G(1,4)\frac{G^{-1}(4,5)}{\delta V(3)}G(6,1^+) = i\frac{\delta G(1,1+)}{\delta V(3)}. \tag{4.86}$$

The exchange self-energy $\Sigma_{xc} = \Sigma - \Sigma_H$ can be rewritten in terms of the screened interaction and vertex-function by applying the chain rule to the functional derivative $\delta G^{-1}(4,2)/\delta v(3)$. We obtain

$$\Sigma_{xc}(1,2) = i \int \text{d3d4}\; W(1,3^+)G(1,4)\Gamma(4,2;3). \tag{4.87}$$

This has the same form as the equation (4.72) without the Hartree-Fock part expect the pare interaction is replaced by a screened interaction. The polarization propagator can also be written with help of the vertex function

$$P(1,2) = -i \int \text{d3d4 } G(2,3)G(4,2^+)\Gamma(3,4;1). \tag{4.88}$$

We can now generate expansion to the Γ, Σ_{xc} and P terms in W. For example zeroth order in W gives

$$\Gamma^{(0)}(1,2;3) = \delta(1,2)\delta(1,3) \tag{4.89}$$
$$P^0(1,2) = -iG(2,1)G(1,2^+) \tag{4.90}$$
$$\Sigma^{(1)}_{xc}(1,2) = iW(1^+,2)G(1,2) \tag{4.91}$$

and first order in W gives following equations

$$\Gamma^{(1)}(1,2;3) = iW(1^+,2)G(1,2)G(3,2) \tag{4.92}$$
$$P^1(1,2) = -i^2 \int \text{d3d4 } G(2,3)G(4,2^+)W(3^+,4)g(3,1)G(1,4) \tag{4.93}$$
$$\Sigma^{(2)}_{xc}(1,2) = i^2 \int \text{d3d4 } W(1^+,2)G(1,4)W(4^+,2)G(4,3)G(3,2) \tag{4.94}$$

Continuing this way we can generate infinite partial summations in W. Because all the quantities W, Σ and P are functionals of the Green function, these equations have to be solved self-consistently with the equation of motion.

The first oder approximation for the screened interaction is

$$W_0(1,2) = w(1,2) = i \int \text{d3d4 } w(1,3)P_0(3,4)W_0(4,2), \tag{4.95}$$

which is the Dyson equation for the screened interaction. This can be solved by repeated substitution like the Dyson equation for the one-particle Green function. Writing it formally open

$$W = w + wP_0W_0 = w + wP_0w + wP_0wP_0w + ... \tag{4.96}$$

If we substitute this in to the equation of self-energy Σ with the definition of the polarization propagator P_0 we get

$$\begin{aligned} \Sigma^{(1)}_{xc}(1,2) &= iw(1,2)G_0(1,2) \\ +i \int \text{d3d4 } & w(1,3)G_0(3,4)G_0(4,1)w(4,2)G_0(1,2) + .. \,, \end{aligned} \tag{4.97}$$

which contains second and higher order terms in the expansion of the self-energy in the bare interaction. The use of screened interaction therefore picks a selected set of self-energy terms and sums them up to finite order. The particles in the interacting system respond to the potential, which includes the induced potential due to the response of the system to the external potential.

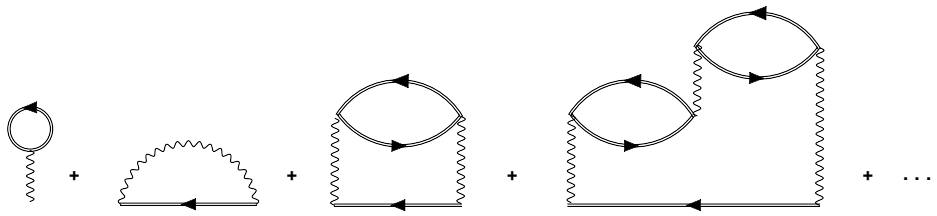

Figure 4.6: GW approximation self-energy (Feynman) diagrams.

4.3 Conserving approximations

For a given self-energy approximation we can define the Green function from the Dyson equation or from the Kadanoff-Baym equations. From the obtained Green function we can calculate all the single-particle expectation values like current. It is important that these quantities obey the fundamental conservation laws like particle conservation [15] which can be expressed via continuity equation

$$\partial_t n(\mathbf{r}, t) = -\nabla \cdot \mathbf{j}(\mathbf{r}, t). \tag{4.98}$$

If the self-energy is obtained from some approximate Φ-functional according to

$$\Sigma(1,2) = \frac{\delta \Phi[G]}{\delta G(2,1)}, \tag{4.99}$$

then the calculated observables satisfy the macroscopic conservation laws. This was proven by Baym [12, 13]. Luttinger and Ward showed that this kind of functional could be constructed by summing over irreducible self-energy diagrams closed with additional Green function line (k labels the Σ-diagrams and n labels the number of interaction lines)

$$\Phi[G] = \sum_{n,k} \frac{1}{2n} \int \mathrm{d1d2}\ \Sigma_k^{(n)}(1,2) G(2,1^+) = \sum_{n,k} \frac{1}{2n} \mathrm{tr}\left[\Sigma_k^{(n)} G\right]. \tag{4.100}$$

To derive the continuity equation from the Green function formalism [12, 13, 16] we need the expectation values of the density and current density operator in terms of the Green function

$$\langle \hat{n}(1) \rangle = iG(1,1^+), \tag{4.101}$$

$$\langle \hat{\mathbf{j}}(1) \rangle = -i \left\{ \left[\frac{\nabla_1}{2i} - \frac{\nabla_{1^+}}{2i} \right] G(1,1^+) \right\}_{1'=1^+}. \tag{4.102}$$

From the equations of motion of the Green function

$$\left[i\partial_1 - \hat{h}(1)\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\, \Sigma(1,3)G(2,3), \tag{4.103}$$

$$\left[-i\partial_2 - \hat{h}(2)\right] G(1,2) = \delta(1,2) + \int \mathrm{d}3\, G(1,3)\Sigma(2,3), \tag{4.104}$$

we can derive the condition that must be satisfied for the particle conservation (continuity equation). By subtracting previous equations and letting $2 \to 1^+$ we obtain

$$\begin{aligned} &\left[i\partial_1 + i\partial_{1^+} - \hat{h}(1) + \hat{h}(1^+)\right] G(1,1^+) \\ &= \int d\bar{1} \left[\Sigma(1,\bar{1})G(\bar{1},1^+) - G(1,\bar{1})\Sigma(\bar{1},1^+)\right]. \end{aligned} \tag{4.105}$$

If the integral in the right hand side is zero, we have

$$\left[i\partial_1 + i\partial_{i^+}\right] G(1,1^+) = [\hat{h}(1) - \hat{h}(1^+)]G(1,1^+) \tag{4.106}$$

which reduces to

$$\left[i\partial_1 + i\partial_{i^+}\right] G(1,1^+) = [(\nabla_1 + \nabla_{1^+})(\nabla_1 - \nabla_{1^+})]G(1,1^+), \tag{4.107}$$

which then gives

$$\partial_1 \langle \hat{n}(1) \rangle = -\nabla_1 \langle \mathbf{j}(1) \rangle. \tag{4.108}$$

Therefore the continuity equation is satisfied provided that

$$\int d\bar{1} \left[\Sigma(1,\bar{1})G(\bar{1},1^+) - G(1,\bar{1})\Sigma(\bar{1},1^+)\right] = 0. \tag{4.109}$$

The continuity equation or number conservation follows from the gauge invariance of $\Phi[G]$. By performing a gauge transformation

$$\mathbf{A} \to \mathbf{A}' + \nabla\lambda(1), \tag{4.110}$$

$$\mathbf{v} \to \mathbf{v}' + \partial_{t_1}\lambda(1), \tag{4.111}$$

where the vector potential $\mathbf{A}$ is written only for convenience although in this derivation it is taken to be zero. The λ is a arbitrary function which satisfies the boundary condition $\lambda(t_0) = \lambda(t_0 - i\beta)$. Under this transformation the Hamiltonian is

$$\hat{h}' = \frac{1}{2}[\nabla + \nabla\lambda]^2 + v' + \partial_t\lambda - \mu. \tag{4.112}$$

The Green function has to be transformed such as it satisfies the equation of motion with the transformed Hamiltonian

$$(i\partial_{t_1} - \hat{h}')G(1,2;\lambda) = \delta(1,2) + \int \mathrm{d}3\, \Sigma(1,3;\lambda)G(3,2;\lambda). \tag{4.113}$$

Starting from the noninteracting Green function, which satisfies the following equation

$$(i\partial_{t_1} - \hat{h}')G_0(1,2;\lambda) = \delta(1,2), \tag{4.114}$$

it can be seen that the noninteracting Green function need to transform as

$$G_0(1,2;\lambda) \to e^{-i\lambda(1)}G_0(1,2)e^{i\lambda(2)}. \tag{4.115}$$

This can be seen by direct differentiation or by looking how the wave functions change under the gauge transformation and the defining the transformed field operators and defining the transformed Green function with these operators.

Using the equation (4.115) and Dyson equation for interacting Green function it is seen that the interacting Green function and self-energy need also transform as

$$G(1,2;\lambda) \to e^{-i\lambda(1)}G(1,2)e^{i\lambda(2)} \tag{4.116}$$
$$\Sigma(1,2;\lambda) \to e^{-i\lambda(1)}\Sigma(1,2)e^{i\lambda(2)} \tag{4.117}$$

which also follows from the particle conservation in the vertices [12, 13]. The change in $\Phi[G]$ when Green function is changed by δG is [16]

$$\delta\Phi[G] = \mathrm{Tr}\left\{\Sigma\delta G\right\} = \int \mathrm{d1d2}\,\Sigma(1,2)\delta G(2,1). \tag{4.118}$$

From the equation (4.116) the firs order change in G with respect to λ is

$$\delta G(1,2) = -i(\lambda(1) - \lambda(2))G(1,2) \tag{4.119}$$

and therefore

$$\begin{aligned}\delta\Phi[G] &= -i\int\int \mathrm{d1d2}\,\Sigma(1,2)(\lambda(2) - \lambda(1))G(2,1) \\ &= i\int\int \mathrm{d1d2}\,[\Sigma(1,2)G(2,1) - G(1,2)\Sigma(2,1)]\lambda(1)\end{aligned} \tag{4.120}$$

this has to be true for all λ and thus

$$\int \mathrm{d2}\,[\Sigma(1,2)G(2,1) - G(1,2)\Sigma(2,1)] = 0, \tag{4.121}$$

which implies the validity of continuity equation. The continuity equation is therefore consequence of the gauge invariance of the $\Phi[G]$ with the condition (4.99) satisfied.

The momentum conservation follows from the invariance of $\Phi[G]$ under translations whereas the angular momentum conservation is consequence of the invariance of $\Phi[G]$ under rotations. The energy conservation follows from the invariance of $\Phi[G]$ when observer uses a flexible clock [12, 13].

5 Steady state current

5.1 Steady-state current directly from model Hamiltonian

At the beginning when people started to study quantum transport with Green function techniques, the system were divided into three different partition; left lead, central region and right lead [17, 18], each with their own electrochemical potentials. At a given time t_0 these three distinct parts are connected and the system reaches a non-equilibrium steady state.

The system is described by a similar Hamiltonian as in the previous case, but the the operators in the leads and central region belong to different spaces. Thus the Hamiltonian can be broken into three pieces $H = H_{\text{cen}} + H_c + H_{\text{cen,int}} + H_t$

$$\begin{aligned}\hat{\mathrm{H}}(t) = \sum_{l\sigma} \epsilon_{ll}(t)\hat{c}^\dagger_{l\sigma}\hat{c}_{l\sigma} + \sum_{k\alpha}[\epsilon_{k\alpha k\alpha} + U_\alpha(t)]\hat{c}^\dagger_{k\alpha\sigma}\hat{c}_{k\alpha\sigma} + \frac{1}{2}\sum_{ij,mn;\sigma} w_{ij,mn}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{m\sigma'}\hat{c}_{j\sigma'}\hat{c}_{n\sigma} \\ + \sum_{lk\alpha\sigma}[V_{k\alpha,l}\hat{c}^\dagger_{k\alpha\sigma}\hat{c}_{l\sigma} + V_{l,k\alpha}\hat{c}^\dagger_{l\sigma}\hat{c}_{k\alpha\sigma}].\end{aligned} \tag{5.1}$$

where H_{cen} describes the central region, $H_{\text{cen,int}}$ interactions in the central region, H_c the contacts and H_t coupling between the leads and the central region. In the following the diagonal terms are denoted for simplicity by one index only.

The current through left lead is by definition the ensemble averaged time derivative of the number operator

$$I_\alpha(t) = \left\langle \frac{\mathrm{d}}{\mathrm{d}t}\hat{N}_\alpha \right\rangle = i\left\langle \left[\hat{H}, \hat{N}_\alpha\right] \right\rangle. \tag{5.2}$$

The definition for the number operator is $\hat{N}_\alpha = \sum_k \hat{c}^\dagger_{k\alpha}\hat{c}_{k\alpha}$. Because the creation and annihilation operators in the leads and in the central region belong to the different Hilbert spaces, the commutator between the central region and interaction parts of the Hamiltonian vanish. Because the lead part of the Hamiltonian is proportional to the number operator in the lead, the commutator between the led Hamiltonian and

the number operator vanish. Only contribution to the current comes from the coupling part of the Hamiltonian and it is found to be

$$I_\alpha^\infty = \sum_{lk} \left[V_{k\alpha,l} \langle c_{k\alpha}^\dagger c_l \rangle - V_{l,k\alpha} \langle c_l^\dagger c_{k\alpha} \rangle \right]. \tag{5.3}$$

To proceed we define the greater and lesser Green functions as

$$G_{l,k\alpha}^<(t,t') = i\langle c_{k\alpha}^\dagger(t) c_l(t') \rangle, \tag{5.4}$$

$$G_{l,k\alpha}^>(t,t') = -i\langle c_l(t') c_{k\alpha}^\dagger(t) \rangle, \tag{5.5}$$

these are related through the relation $G_{k\alpha,l}^<(t,t) = -[G_{k\alpha,l}^>(t,t)]^*$. The current can therefore be written as

$$I_\alpha^\infty = 2\mathrm{Re}\left[\sum_{kl} V_{l,k\alpha} G_{k\alpha,l}^<(t,t) \right]. \tag{5.6}$$

Next thing is to find an equation for $G_{C\alpha}^<(t,t)$. This can be done as in chapter 3 by calculating the commutator $[\hat{c}_s(t), H]$ and multiplying by $\hat{c}_{k\alpha}^\dagger(t')$, time-ordering the operators and taking the ensemble average. The last step is to identify the Green functions and the result is

$$[i\partial_t - \varepsilon_{k\alpha}(t)] G_{k\alpha,l'}(t,t') = \sum_l V_{l,k\alpha} G_{ll'}(t,t'). \tag{5.7}$$

Defining the lead Green function $g_{k\alpha}$ which satisfies the equation $(i\partial_t - \varepsilon_{k\alpha}) g_{k\alpha}(t,t') = \delta(t,t')$ we are able to write a Dyson equation for $G_{k\alpha,l}(t,t')$ as

$$G_{k\alpha,l'}(t,t') = \sum_l \int \mathrm{d}\bar{t}\, V_{k\alpha,l} G_{ll'}(t,\bar{t}) g_{k\alpha}(\bar{t},t'). \tag{5.8}$$

Using the Langreth-rules [19] or proceeding in the same way as in chapter 3 we get the equation for $G_{k\alpha,l'}^<(t,t')$ to be of the form

$$G_{k\alpha,l'}^<(t,t') = \sum_l \int \mathrm{d}\bar{t}\, V_{k\alpha,l} \left[G_{ll'}^R(t,\bar{t}) g_{k\alpha}^<(\bar{t},t') + G_{ll'}^<(t,\bar{t}) g_{k\alpha}^A(\bar{t},t') \right]. \tag{5.9}$$

Inserting this equation to the equation of current

$$I_\alpha^\infty = 2\mathrm{Re}\left\{ \sum_{kll'} V_{l',k\alpha} \int \mathrm{d}\bar{t}\, V_{k\alpha,l} \left[G_{ll'}^R(t,\bar{t}) g_{k\alpha}^<(\bar{t},t') + G_{ll'}^<(t,\bar{t}) g_{k\alpha}^A(\bar{t},t') \right] \right\} \tag{5.10}$$

and using the definitions of the lead Green functions

$$g_{k\alpha}^<(t,t') = if(\varepsilon_{k\alpha}) e^{-i\int_{t'}^t d\bar{t}\varepsilon_{k\alpha}(\bar{t})}, \tag{5.11}$$

$$g_{k\alpha}^A(t,t') = i\theta(t'-t) e^{-i\int_{t'}^t d\bar{t}\varepsilon_{k\alpha}(\bar{t})}, \tag{5.12}$$

then we have

$$I_\alpha^\infty = 2\mathrm{Re}\left\{ \sum_{ll'k} i \int \mathrm{d}t\; e^{-i\int_t^{\bar{t}}\, \mathrm{d}t\varepsilon_{k\alpha}(t)} \left[G^R_{ll'}(t,\bar{t}) f(\varepsilon_{k\alpha}) + \theta(\bar{t}-t) G^<_{ll'}(t,\bar{t}) \right] \right\}. \quad (5.13)$$

Defining the level broadening or level width function as ($\varepsilon_{k\alpha}(t) = \varepsilon_{k\alpha} - U_{k\alpha}(t)$)

$$\Gamma_{ll'}(\varepsilon, t', t) = 2\pi \sum_k \delta(\varepsilon - \varepsilon_{k\alpha}) V_{k\alpha,l} V_{l',k\alpha} e^{-i\int_{t'}^{t} d\bar{t} U_{k\alpha}(\bar{t})} \quad (5.14)$$

we obtain a following equation for steady-state current

$$I_\alpha^\infty = -2\mathrm{Im}\left\{ \sum_{ll'} \int_{-\infty}^{t} \mathrm{d}\bar{t} \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(\bar{t}-t)} \Gamma^\alpha_{ll'}(\varepsilon, \bar{t}, t) \times \left[G^<_{ll'}(t,\bar{t}) + G^R_{ll'}(t,\bar{t}) f_\alpha(\varepsilon) \right] \right\}. \quad (5.15)$$

This equation appears in the paper of Jauho, Meir and Wingreen [18]. They prove that in the time-independent limit when the line width $\mathbf{\Gamma}$ depends only on the energy this equation becomes

$$I_\alpha^\infty = i \int \frac{\mathrm{d}\varepsilon}{2\pi} \mathrm{Tr}\left\{ \mathbf{\Gamma}_\alpha(\varepsilon) \left[\mathbf{G}^<(\varepsilon) + f_\alpha(\varepsilon) \left(\mathbf{G}^R(\varepsilon) - \mathbf{G}^A(\varepsilon) \right) \right] \right\}, \quad (5.16)$$

which can be symmetrized to get the usual Meir-Wingreen formula [17].

5.2 Steady-state current from the Keldysh formalism

Next it is shown how the steady-state equation for the current, *i.e*, the Meir-Wingreen [17] equation is reached from the Keldysh formalism. Starting from the equation

$$\begin{aligned} I_\alpha(t) = -2\mathrm{Re}\Bigg\{ \mathrm{Tr}_\mathrm{C}\Bigg[\int_0^\infty \mathrm{d}\bar{t} [\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t}) \mathbf{\Sigma}^A_{\alpha,\mathrm{em}}(\bar{t},t) + \mathbf{G}^R_{\mathrm{CC}}(t,\bar{t}) \mathbf{\Sigma}^<_{\alpha,\mathrm{em}}(\bar{t},t)] \\ + \int_0^{-i\beta} d\bar{\tau} \mathbf{G}^\rceil_{\mathrm{CC}}(t,\bar{\tau}) \mathbf{\Sigma}^\lceil_{\alpha,\mathrm{em}}(\bar{\tau},t) \Bigg] \Bigg\} \end{aligned} \quad (5.17)$$

and taking the limit $t \to \infty$. Assuming also that in this limit the Green function depends only on the difference of its time arguments, and that the Green function and self-energy vanishes if the separation between its time arguments goes to infinity. By also using the definition of the embedding self-energy we have

$$\begin{aligned} I_\alpha^\infty = 2\mathrm{Re}\Bigg\{ \mathrm{Tr}_\mathrm{C}\Bigg[\int_0^\infty \mathrm{d}\bar{t} [\mathbf{G}^<_{\mathrm{CC}}(t,\bar{t}) \mathbf{H}_{\mathrm{C}\alpha} \mathbf{g}^A_{\alpha\alpha}(\bar{t},t') \mathbf{H}_{\alpha\mathrm{C}} \\ + \mathbf{G}^R_{\mathrm{CC}}(t,\bar{t}) \mathbf{H}_{\mathrm{C}\alpha} \mathbf{g}^<_{\alpha\alpha}(\bar{t},t) \mathbf{H}_{\alpha\mathrm{C}}] \Bigg] \Bigg\}. \end{aligned} \quad (5.18)$$

Using the definitions of the lead Green functions

$$\mathbf{g}_\alpha^<(t,t') = if(\mathbf{E}_\alpha)e^{-i\int_{t'}^t d\bar{t}\mathbf{E}_\alpha(\bar{t}),} \tag{5.19}$$

$$\mathbf{g}_\alpha^A(t,t') = i\theta(t'-t)e^{-i\int_{t'}^t d\bar{t}\mathbf{E}_\alpha(\bar{t})}, \tag{5.20}$$

and writing the matrices by using, indices we end up to a same equation as before (Eq. (5.13))

$$I_\alpha^\infty = 2\mathrm{Re}\Bigg\{\sum_{ll'k} i\int \mathrm{d}t\; e^{-i\int_t^{\bar{t}}\mathrm{d}t'\varepsilon_{k\alpha}(t')}V_{l,k\alpha}V_{k\alpha,l}\Big[G_{ll'}^R(t,\bar{t})f(\varepsilon_{k\alpha}) + \theta(\bar{t}-t)G_{ll'}^<(t,\bar{t})\Big]\Bigg\}. \tag{5.21}$$

The definition of the level broadening or level width function is as in equation (5.14). Then the following equation for steady-state current is obtained

$$\begin{aligned} I_\alpha^\infty = -2\mathrm{Im}\Bigg\{\sum_{ll'}\int_{-\infty}^t \mathrm{d}\bar{t}\int\frac{d\varepsilon}{2\pi}e^{-i\varepsilon(\bar{t}-t)}\Gamma_{ll'}^\alpha(\varepsilon,\bar{t},t) \\ \times\left[G_{ll'}^<(t,\bar{t}) + G_{ll'}^R(t,\bar{t})f_\alpha(\varepsilon)\right]\Bigg\}. \end{aligned} \tag{5.22}$$

which equals to equation (5.15). Therefore, the steady-state current given by Kadanoff-Baym approach and Keldysh techniques equals the Meir-Wingreen steady state.

5.3 The non-interacting resonant level model

In this section the non-interacting resonant level model is studied. The analysis is based on the article by Gianluca Stefanucci [10]. The resonant tunneling system is a first approximation for a semiconductor heterostructure coupled to two metallic leads. The metallic leads are the electron reservoirs. In this derivation we consider a system of non-interacting electrons described by Hamiltonian

$$\hat{H}_0 = \sum_{mn} T_{mn}\hat{c}_m^\dagger\hat{c}_n \quad , \quad (\bar{T})_{mn} = T_{mn}, \tag{5.23}$$

$$\hat{H}_U = \sum_{mn} U_{mn}(t)\hat{c}_m^\dagger\hat{c}_n \quad , \quad [\bar{U}(t)]_{mn} = U_{mn}(t), \tag{5.24}$$

where $\hat{H}_U$ describes a time-dependent disturbance.

First we need an expression for the lesser Green function which is the key quantity when calculating the current. . We start by defining the Hamiltonian as

$$H(t) = H_0 + H_U(t) = \sum_m \varepsilon_m(t)\hat{c}_m^\dagger\hat{c}_m + \sum_{mn} V_{mn}(t)\hat{c}_m^\dagger\hat{c}_n, \tag{5.25}$$

where $\varepsilon_{mn}(t)$ describes the on-site energy of the levels and V_{mn} is the off-diagonal hopping element. The operators $\hat{c}^\dagger$, $\hat{c}$ are the usual creation and annihilation operators. The equation of motion for the Green function reads now

$$i\partial_t \mathbf{G}(z,z') = \delta(z,z') + \mathbf{H}(z)\mathbf{G}(z). \tag{5.26}$$

In a similar way we can derive also the adjoint for the equation of motion

$$\left[-i\partial_{z'} - \mathbf{H}(z)\right]\mathbf{G}(z,z') = \delta(z,z'). \tag{5.27}$$

We will also need the greater / lesser and retarded / advanced components of the lead Green function which has been derived already earlier. These components of the lead Green function read as

$$\mathbf{g}^<(z,z') = if(\boldsymbol{\mathcal{E}})e^{-i\int_{z'}^{z} \mathrm{d}\bar{z}\,\boldsymbol{\mathcal{E}}(\bar{z})}, \tag{5.28}$$

$$\mathbf{g}^>(z,z') = i[f(\boldsymbol{\mathcal{E}})-1]e^{-i\int_{z'}^{z} \mathrm{d}\bar{z}\boldsymbol{\mathcal{E}}(\bar{z})}, \tag{5.29}$$

$$\mathbf{g}^{R,A}(t,t') = \mp\theta(\pm t \mp t')e^{-i\int_{t'}^{t} \mathrm{d}\bar{t}\boldsymbol{\mathcal{E}}(t)}. \tag{5.30}$$

The uncontacted Green function or the lead Green function allows us to write

$$\begin{aligned}\left[i\partial_{\bar{z}} - \boldsymbol{\mathcal{E}}(\bar{z}) - \mathbf{V}(\bar{z})\right]\mathbf{G}(\bar{z},z') &= \delta(\bar{z},')\Big|\cdot\int \mathrm{d}\bar{z}\mathbf{g}(z,\bar{z}) \\ \int \mathrm{d}\bar{z}\mathbf{g}(z,\bar{z})\left[i\partial_{\bar{z}} - \boldsymbol{\mathcal{E}}(\bar{z}) - \mathbf{V}(\bar{z})\right]\mathbf{G}(\bar{z},z') &= \mathbf{g}(z,z')\end{aligned} \tag{5.31}$$

the equation of motion in the integral form

$$\mathbf{G}(z,z') = \mathbf{g}(z,z') + \int \mathrm{d}\bar{z}\mathbf{g}(z,\bar{z})\mathbf{V}(\bar{z})\mathbf{G}(\bar{z},z'). \tag{5.32}$$

By using the Langreth rules [20] we can extract the greater and lesser components of the Green function.

$$\mathbf{G}^< = \mathbf{g}^<\cdot(\delta + \mathbf{V}\cdot\mathbf{G}^A) + \mathbf{g}^R\cdot\mathbf{V}\cdot G^< + \mathbf{g}^\rceil\star\mathbf{V}\star\mathbf{G}^\lceil, \tag{5.33}$$

$$\mathbf{G}^> = \mathbf{g}^>\cdot(\delta + \mathbf{V}\cdot\mathbf{G}^A) + \mathbf{g}^R\cdot\mathbf{V}\cdot\mathbf{G}^> + \mathbf{g}^\rceil\star\mathbf{V}\star\mathbf{G}^\lceil, \tag{5.34}$$

where we have introduced the following short hand notation

$$\star = i\int_0^\beta \mathrm{d}\tau \qquad\qquad \cdot = \int_0^\infty \mathrm{d}.t \tag{5.35}$$

We can get an expression for the retarded and advanced component of the Green function (see Appedinx G) Now we solve the equations (5.33) and (5.34) for $\boldsymbol{G}^{\gtrless}$

$$\mathbf{G}^{\gtrless} = (\delta + \mathbf{V}\cdot\mathbf{G}^A)\cdot\mathbf{g}^{\gtrless}\cdot(\delta + \mathbf{V}\cdot\mathbf{G}^A) + (\delta + \mathbf{V}\cdot\mathbf{G}^A)\cdot\mathbf{g}^\rceil\star\mathbf{V}\star\mathbf{G}^\lceil. \tag{5.36}$$

which will eventually lead to (see Appendix G)

$$\mathbf{G}^{\gtrless}(t,t') \;=\; \mathbf{G}^{R}(t,0)\mathbf{G}^{\gtrless}(0,0)\mathbf{G}^{A}(0,t'). \tag{5.37}$$

Now if we include interactions and the full Hamiltonian is

$$\hat{H} = \sum_{m} \varepsilon_m(t)\bar{c}_m c_m + \sum_{mn} V_{mn}(t)\bar{c}_m c_n + \frac{1}{2}\sum_{mn,kl} w_{mn,kl}\bar{c}_m\bar{c}_k c_n c_l \tag{5.38}$$

Now the equation of motion becomes

$$[i\partial_z - \mathbf{h}(z)]\,\mathbf{G}(z,z') \;=\; \delta(z,z') + \int_{\gamma} \mathrm{d}\bar{t}\boldsymbol{\Sigma}[\mathbf{G}](z,\bar{z})\mathbf{G}(\bar{z},z'), \tag{5.39}$$

where $\mathbf{h}(z) = \boldsymbol{\mathcal{E}}(z)+\boldsymbol{V}(z)+\boldsymbol{\Sigma}^{\delta}(z)$. Now we are trying to prove the following equation. The following statement is proved for the lesser function (the greater function is proved in a similar fashion)

$$\mathbf{G}^{\gtrless}(z,z') = \mathbf{G}^{R}(z,0)\mathbf{G}^{\gtrless}(0,0)\mathbf{G}^{A}(0,z') + \boldsymbol{\Delta}^{\gtrless}(z,z'), \tag{5.40}$$

where ($\mathbf{G}^{K} \equiv \mathbf{G}^{>} + \mathbf{G}^{<}$)

$$\begin{aligned}\boldsymbol{\Delta}^{\gtrless}(z,z') = i\mathbf{G}^{R}(z,0)\mathbf{G}^{>}(0,z') - i\mathbf{G}^{<}(z,0)\mathbf{G}^{A}(0,z') - \mathbf{G}^{R}(z,0)\mathbf{G}^{K}(0,0)\mathbf{G}^{A}(0,z') \\ + \left[\mathbf{G}^{R}\cdot\left[\boldsymbol{\Sigma}^{\gtrless} + \boldsymbol{\Sigma}^{\rceil} * \mathbf{G} * \boldsymbol{\Sigma}^{\lceil}\right]\cdot\mathbf{G}^{A}\right](z,z').\end{aligned} \tag{5.41}$$

The Green function can be expressed with help of some reference Green function $\mathbf{G}_0$, which is usually noninteracting Green function, as a Dyson equation

$$\mathbf{G}(z,z') = \mathbf{G}_0(z,z') + \int d\bar{z}d\bar{\bar{z}}\mathbf{G}_0(z,\bar{z})\boldsymbol{\Sigma}(\bar{z},\bar{\bar{z}})\mathbf{G}(\bar{\bar{z}},z). \tag{5.42}$$

The lesser component of the Green function can be obtained by using Langreth theorem

$$\begin{aligned}\mathbf{G}^{<}(z,z') &= \mathbf{G}_0^{<}(z,z') + \int_0^z d\bar{z}\mathbf{G}_0^{R}(z,\bar{z})[\boldsymbol{\Sigma}\mathbf{G}]^{<}(\bar{z},z') \\ &\quad + \int_0^{z'} d\bar{z}\mathbf{G}_0^{<}[\boldsymbol{\Sigma}\mathbf{G}]^{A} + \int_0^{-i\beta} d\tau\mathbf{G}_0^{\rceil}[\boldsymbol{\Sigma}\mathbf{G}]^{\lceil} \\ &= \mathbf{G}_0^{<} + \mathbf{G}_0^{R}\cdot[\boldsymbol{\Sigma}G]^{<} + \mathbf{G}_0^{<}\cdot[\boldsymbol{\Sigma}\mathbf{G}]^{A} + \mathbf{G}^{\rceil}\star[\boldsymbol{\Sigma}\mathbf{G}]^{\lceil},\end{aligned} \tag{5.43}$$

using the Langreth theorem again to the terms $[\boldsymbol{\Sigma}\mathbf{G}]^{\{<,A,\lceil\}}$ we get

$$\begin{aligned}\mathbf{G}^{<} = \mathbf{G}_0(\delta - \mathbf{G}_0\cdot\boldsymbol{\Sigma}^{R}\cdot\mathbf{G}^{A}) + \mathbf{G}_0^{R}\cdot\boldsymbol{\Sigma}^{R}\cdot\mathbf{G}^{<} + (\mathbf{G}_0^{R}\cdot\boldsymbol{\Sigma}^{<} + \boldsymbol{\Sigma}^{\rceil}\star\boldsymbol{\Sigma}^{\lceil})\cdot\mathbf{G}^{A} \\ + \mathbf{G}_0^{R}\cdot\boldsymbol{\Sigma}^{\rceil}\star\mathbf{G}^{\lceil} + \mathbf{G}^{\rceil}\star\boldsymbol{\Sigma}\star\mathbf{G}^{\lceil}.\end{aligned} \tag{5.44}$$

This equation can be solved for $\mathbf{G}^<$. Writing first

$$\begin{aligned}(\delta + \mathbf{G}_0^R \cdot \mathbf{\Sigma}^R)\mathbf{G}^< = \mathbf{G}_0(\delta - \mathbf{\Sigma}^R \cdot \mathbf{G}^A) + (\mathbf{G}_0^R \cdot \mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil \star \mathbf{\Sigma}^\lceil) \cdot \mathbf{G}^A \\ + \mathbf{G}_0^R \cdot \mathbf{\Sigma}^\rceil \star \mathbf{G}^\lceil + \mathbf{G}^\rceil \star \mathbf{\Sigma} \star \mathbf{G}^\lceil.\end{aligned} \tag{5.45}$$

Using the definition of the retarded Green functions $\mathbf{G}^R(z,z') = \theta(z-z')(\mathbf{G}^>(z,z') - \mathbf{G}^<(z,z'))$ the factor in front of $\mathbf{G}^>$ can be expressed as $(\delta - \mathbf{G}_0^R \cdot \mathbf{\Sigma}^R)) = \mathbf{G}_0^R(\mathbf{G}^R)^{-1}$. For example

$$\begin{aligned}\mathbf{G}^> - \mathbf{G}^< = (\mathbf{G}_0^> - \mathbf{G}_0^<)(\delta + \mathbf{\Sigma}^A \cdot \mathbf{G}^A) + \mathbf{G}_0^R \cdot \mathbf{\Sigma}^R \cdot \mathbf{G}^< + \mathbf{G}_0^R \mathbf{\Sigma}^< \mathbf{G}^A \\ = \mathbf{G}_0^R(\delta + \mathbf{\Sigma}^R \mathbf{G}^R).\end{aligned} \tag{5.46}$$

Then we have

$$\begin{aligned}\mathbf{G}_0^R(\mathbf{G}^R)^{-1}\mathbf{G}^< = \mathbf{G}_0(\delta - \mathbf{G}_0 \cdot \mathbf{\Sigma}^R \cdot \mathbf{G}^A) + (\mathbf{G}_0^R \cdot \mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil \star \mathbf{\Sigma}^\lceil) \cdot \mathbf{G}^A \\ + \mathbf{G}_0^R \cdot \mathbf{\Sigma}^\rceil \star \mathbf{G}^\lceil + \mathbf{G}^\rceil \star \mathbf{\Sigma} \star \mathbf{G}^\lceil.\end{aligned} \tag{5.47}$$

Multiplying this equation from the right with $(\mathbf{G}_0^R)^-1\mathbf{G}^R$ which is according to Dyson equation same as $\delta + \mathbf{\Sigma}^R\mathbf{G}^R$ we get

$$\begin{aligned}\mathbf{G}^< = (\delta + \mathbf{\Sigma}^R\mathbf{G}^R)\mathbf{G}_0^<(\delta - \mathbf{\Sigma}^R \cdot \mathbf{G}^A) + (\delta + \mathbf{\Sigma}^R\mathbf{G}^R)(\mathbf{G}_0^R \cdot \mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil \star \mathbf{\Sigma}^\lceil) \cdot \mathbf{G}^A \\ + (\delta + \mathbf{\Sigma}^R\mathbf{G}^R)(\mathbf{G}_0^R \cdot \mathbf{\Sigma}^\rceil \star \mathbf{G}^\lceil + \mathbf{G}^\rceil \star \mathbf{\Sigma} \star \mathbf{G}^\lceil).\end{aligned} \tag{5.48}$$

Using following identities this equation can be simplified further

$$\mathbf{G}_0^{\gtrless}(t,t') = \mathbf{G}_0^R(t,0)\mathbf{G}_0^{\gtrless}(0,0)\mathbf{G}_0^A(0,t'), \tag{5.49}$$

$$\mathbf{G}_0(\tau,t) = -i\mathbf{G}_0(\tau,0)\mathbf{G}_0^A(0,t), \tag{5.50}$$

$$\mathbf{G}_0(t,\tau) = i\mathbf{G}_0^R(t,0)\mathbf{G}_0(0,\tau). \tag{5.51}$$

we get

$$\mathbf{G}^< = \mathbf{G}^R(z,0)\mathbf{G}^<(0,0)\mathbf{G}^A(0,z). \tag{5.52}$$

Using the Dyson equation for $\mathbf{G}(t,\tau)$ and for $\mathbf{G}(\tau,\tau')$

$$\mathbf{G}(\tau,\tau') = \mathbf{G}_0(\tau,\tau') + [\mathbf{G}_0 \star \mathbf{\Sigma} \star G](\tau,\tau'), \tag{5.53}$$

$$\mathbf{G}(\tau,t) = [\mathbf{G}^R \cdot \mathbf{\Sigma}^\rceil \star G](\tau,t) + i\mathbf{G}^R(t,0)\mathbf{G}(0,\tau), \tag{5.54}$$

$$\mathbf{G}(t,\tau) = [G \star \mathbf{\Sigma}^\lceil \cdot \mathbf{G}^A](t,\tau) - i\mathbf{G}(\tau,0)\mathbf{G}^A(0,t). \tag{5.55}$$

we end up to an equation

$$\begin{aligned}\mathbf{G}^< = \mathbf{G}^R \cdot \mathbf{G} \cdot \mathbf{G}^A + \mathbf{G}^R \cdot [\mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil \star \mathbf{G} \star \mathbf{\Sigma}^\lceil](z,z') \\ + i\mathbf{G}^R(z,0)[\mathbf{G} \star \mathbf{\Sigma}^\lceil \cdot \mathbf{G}^A](0,z') - i[\mathbf{G}^R \cdot \mathbf{\Sigma}^\lceil \star \mathbf{G}](z,0)\mathbf{G}^A(0,z').\end{aligned} \tag{5.56}$$

With the help of the Dyson equations we can write the last two terms as

$$i\mathbf{G}^R(z,0)[G\star\mathbf{\Sigma}^\ulcorner\cdot\mathbf{G}^A](0,z' = i\mathbf{G}^R(z,0)\mathbf{G}^>(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^>(0,0)\mathbf{G}^A(0,z') \quad (5.57)$$

and

$$-i[\mathbf{G}^R\cdot\mathbf{\Sigma}^\ulcorner\star G](z,0)\mathbf{G}^A(0,z') = -i\mathbf{G}^<(z,0)\mathbf{G}^A(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^<(0,0)\mathbf{G}^A(0,z'). \quad (5.58)$$

This leads us to the final result

$$\begin{aligned}\mathbf{G}^\gtrless(z,z') &= \mathbf{G}^R(z,0)\mathbf{G}^\gtrless(0,0)\mathbf{G}^A(0,z') + i\mathbf{G}^R(z,0)\mathbf{G}^>(0,z') \\ &\quad -i\mathbf{G}^<(z,0)\mathbf{G}^A(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^K(0,0)\mathbf{G}^A(0,z') \\ &\quad + \left[\mathbf{G}^R\cdot\left[\mathbf{\Sigma}^\gtrless + \mathbf{\Sigma}^\urcorner * G * \mathbf{\Sigma}^\ulcorner\right]\cdot\mathbf{G}^A\right](z,z') \\ &= \mathbf{G}^R(z,0)\mathbf{G}^\gtrless(0,0)\mathbf{G}^A(0,z') + \mathbf{\Delta}^\gtrless(z,z'). \quad (5.59)\end{aligned}$$

If the Green functions vanish when the separation between their time-variables goes to infinity we get

$$\lim_{t,t'\to\infty}\boldsymbol{G}^\gtrless(t,t') = [\boldsymbol{G}^R\cdot\mathbf{\Sigma}^\gtrless\cdot\boldsymbol{G}^A](t,t'). \quad (5.60)$$

This equation is convenient for studying the long-time response of an interacting system under an external time-dependent perturbation.

5.3.1 Noninteracting resonant tunneling systems

Now we study the time-dependent current response through a noninteracting resonant tunneling system. The system is described by the Hamilronian

$$H_0 = \sum_{k\alpha}\varepsilon_{k\alpha}c^\dagger_{k\alpha}c_{k\alpha} + \varepsilon_0 c^\dagger_0 c_0 + \sum_{k\alpha}V_{k\alpha}[c^\dagger_{k\alpha}c_0 + c^\dagger_0 c_{k\alpha}] \equiv \sum_{mn}T_{mn}c^\dagger_m c_n, \quad (5.61)$$

where m,n=collective indices for $k\alpha$ and 0. m α = L,R denotes the left or right lead. The system is perturbed by the perturbation

$$H_U(t) = \sum_{k\alpha}U_{k\alpha}(t)c^\dagger_{k\alpha}c_{k\alpha} + U_0(t)c^\dagger_0 c_0 \equiv \sum_{mn}U_{mn}(t)c^\dagger_m c_n. \quad (5.62)$$

Before the perturbation the system is at thermodynamic equilibrium. The current through the α contact can be calculated from the time derivative of the of the occupation number operator N_α of the α contact. The current is defined as

$$\begin{aligned}I_\alpha(t) &= -e\int_\alpha d\boldsymbol{r}\frac{d}{dt}n(\boldsymbol{r},t) \quad (5.63)\\ &= 2e\sum_k \mathrm{Re}[G^<_{0,k\alpha}(t,t)]V_{k\alpha} \\ &= 2e\sum_k \mathrm{Re}[\boldsymbol{G}^R(t,0)\boldsymbol{G}^<(0,0)\boldsymbol{G}^A(0,t)]_{0,k\alpha}V_{k\alpha}. \quad (5.64)\end{aligned}$$

The matrix $\mathbf{G}^<(0,0)$ can be written as

$$\begin{aligned}\mathbf{G}^<(0,0) &= \frac{i}{e^{\beta H}+1} = \frac{i}{e^{\beta(\varepsilon-V)}+1} && (5.65)\\ &= \int_\gamma \frac{\mathrm{d}z}{2\pi}\frac{1}{z-H}\frac{e^{\eta\xi}}{e^{\beta\xi}+1} && (5.66)\\ &= \int_\gamma \frac{\mathrm{d}\xi}{2\pi}\frac{1}{\xi-\varepsilon-V}\frac{e^{\eta\xi}}{e^{\beta\xi}+1}. && (5.67)\end{aligned}$$

The poles areat $\xi = \varepsilon - V$. The factor $e^{\eta\xi}$ ensures the convergence, integrand $\to 0$ faster than $1/|z|$ when $|z| \to \infty$. Now the current through the contact α can be written as

$$\begin{aligned}I_\alpha(t) &= 2e\sum_k \mathrm{Re}\left\{\left[\mathbf{G}^R(t,0)\mathbf{G}^<(0,0)\mathbf{G}^A(0,t)\right]_{0,k\alpha} V_{k\alpha}\right\}\\ &= 2e\sum_k \mathrm{Re}\left\{\left[\mathbf{G}^R(t,0)\int_\Gamma \frac{d\xi}{2\pi}\frac{f(\xi)e^{\eta\xi}}{\xi-\varepsilon-V}\mathbf{G}^A(0,t')\right]_{k\alpha} V_{k\alpha}\right\}\\ &= 2e\mathrm{Re}\left\{\int_\Gamma \frac{\mathrm{d}\xi}{2\pi} f(\xi)^{\eta\xi}\sum_k\left[\mathbf{G}^R(t,0)\frac{1}{\xi-\mathrm{E}-\mathbf{V}}\mathbf{G}^A(0,t')\right]_{0,k\alpha} V_{k\alpha}\right\}\\ &= 2e\mathrm{Re}\left\{\int_\Gamma \frac{\mathrm{d}\xi}{2\pi} f(\xi)^{\eta\xi}\mathbf{Q}_\alpha(\xi,t)\right\}, \qquad (5.68)\end{aligned}$$

where $\mathbf{Q}_\alpha(\xi,t) = \sum_k \left[\mathbf{G}^R(t,0)\boldsymbol{G}(\xi)\mathbf{G}^A(0,t')\right]_{0,k\alpha} V_{k\alpha}$.

Step-like modulation

$U_{k\alpha} = U_{alpha}$: Steady-state current

To keep things simple we look now only a step-like modulation where the bias voltage is given as

$$U_{mn}(t) = \theta(t)U_{mn}. \qquad (5.69)$$

From the equation

$$G^{R,A}(t,t') = \mp(\pm t \mp t')S(t)S^\dagger(t') \Rightarrow G^R(t,0) = -i\theta(t)S(t) \qquad (5.70)$$

where $(H = \boldsymbol{\mathcal{E}} + \boldsymbol{V} + U)$

$$S_{mn}(t) = -\delta_{mn}e^{-i\int_0^t d\bar{t}H(\bar{t})} \qquad (5.71)$$

it follows that

$$\boldsymbol{G}^R(t,0) = -i\theta(t)e^{-i\int_0^t d\bar{t}(\boldsymbol{\mathcal{E}}+\boldsymbol{V}+U)} \equiv \int \frac{d\omega}{2\pi}e^{-i\omega t}\boldsymbol{G}^R(\omega). \qquad (5.72)$$

Since $[\boldsymbol{G}^R(t,0)]^\dagger = \boldsymbol{G}^A(0,t)$ The device component of $G^{R,A}(\omega)$ is

$$G^{R,A}(\omega) = \frac{1}{\omega - \tilde{\varepsilon}_0 - \Sigma^{R,A}\omega \pm i\eta}, \tag{5.73}$$

where $\tilde{\varepsilon}_0 = \varepsilon_0 + U_\alpha$ and $\Sigma^{R,A}(\omega) = \sum_\alpha \Sigma^{R,A}_\alpha(\omega) = \sum_\alpha \sum_k \frac{V^2_{k\alpha}}{\omega - \tilde{\varepsilon}_0 \pm i\eta}$ Retarded / advanced self-energy describes the induced by back and forth virtual hopping process from the localized levels to the leads.

The retarded and advanced Green functions obey the equation of motion

$$i\partial_t \boldsymbol{G}^{R,A}(t,t') = \mathbf{1}\delta(t-t') = \boldsymbol{H}(t)\boldsymbol{G}^{R,A}(t,t'). \tag{5.74}$$

Since we are interested what happens after the bias is switched on we set $t' = 0$. The hamiltonian after the bias has switched on is $\hat{H} = \hat{H}_0 + \hat{H}_U$, where $\tilde{\varepsilon}_0 = \varepsilon_0 + U_0$ and $\tilde{\varepsilon}_{k\alpha} = \varepsilon_{k\alpha} + U_{k\alpha}$. The $G^R_{0,0}$ and $G^R_{k\alpha,0}$ components of the retarded Green function are

$$\begin{aligned} i\partial_t G^R_{0,0}(t,0) &= \delta(t) + \tilde{\varepsilon}_0 G^R_{0,0}(t,0) + \sum_{k\alpha} V_{k\alpha} G^R_{k\alpha,0}(t,0), & (5.75)\\ i\partial_t G^R_{k\alpha,0}(t,0) &= \tilde{\varepsilon}_{k\alpha} G^R_{k\alpha,0}(t,0) + V_{k\alpha} G^R_{0,0}(t,0). & (5.76) \end{aligned}$$

These Green functions can be calculated by introducing the uncontacted Green function.

$$\begin{aligned} (i\partial_t - \tilde{\varepsilon}_0) g^R_0(t) &= \delta(t), & (5.77)\\ (i\partial_t - \tilde{\varepsilon}_{k\alpha}) g^R_{k\alpha}(t) &= \delta(t). & (5.78) \end{aligned}$$

Then we get a Dyson like expressions for the $G^R_{0,0}$ and $G^R_{k\alpha,0}$ components of the retarded Green function

$$\begin{aligned} G^{R,A}_{k\alpha,0}(t,0) &= V_{k\alpha} \int_{-\infty}^{\infty} dt' g^{R,A}_{k\alpha}(t-t') G^{R,A}_{0,0}(t,0), & (5.79)\\ G^{R,A}_{0,0}(t,0) &= g^{R,A}_0(t) + \sum_{k\alpha} V_{k\alpha} \int_{-\infty}^{\infty} dt' g^{R,A}_0(t-t') G^{R,A}_{k\alpha}(t,0). & (5.80) \end{aligned}$$

By Fourier transforming the uncontacted Green function we get

$$\begin{aligned} g^{R,A}_{k\alpha}(\omega) &= \frac{1}{\omega - \tilde{\varepsilon}_{k\alpha} \pm i\eta}, & (5.81)\\ g^{R,A}_0(\omega) &= \frac{1}{\omega - \tilde{\varepsilon}_0 \pm i\eta}. & (5.82) \end{aligned}$$

The Fourier transform of the $G^{R,A}_{0,0}$ and $G^{R,A}_{k\alpha,0}$ components of the retarded Green function are

$$\begin{aligned} G^{R,A}_{k\alpha,0}(\omega) &= V_{k\alpha} g^{R,A}_{k\alpha}(\omega) G^{R,A}_{0,0}(\omega), & (5.83)\\ G^{R,A}_{0,0}(\omega) &= g^{R,A}_0(\omega) + \sum_{k\alpha} V_{k\alpha} g^{R,A}_0(\omega) G^{R,A}_{0,0}(\omega). & (5.84) \end{aligned}$$

By using the expressions (5.81) and (5.82) we can introduce the self-energy as

$$\Sigma^{R,A}(\omega) = \sum_{\alpha} \Sigma^{R,A}_{\alpha}(\omega) = \sum_{k\alpha} V^2_{k\alpha} g^{R,A}_{k\alpha}(\omega), = \sum_{k\alpha} \frac{V^2_{k\alpha}}{\omega - \tilde{\varepsilon}_{k\alpha} \pm i\eta}. \tag{5.85}$$

The self-energy describes the effects of the leads to the level at the central region.

In the following we will also need the $G_{0,k'\alpha'}$ and $G_{k\alpha,k'\alpha'}$ component of the Green function which satisfies the equations

$$\begin{aligned} G^{R,A}_{0,k\alpha}(\omega) &= G^{R,A}_{0,0}(\omega) V_{k\alpha} g^{R,A}_{k\alpha}(\omega), & (5.86)\\ G^{A}_{k\alpha,k'\alpha'}(\omega) &= \delta_{k\alpha,k'\alpha'} g^{R/A}_{k\alpha}(\omega) + g^{R/A}_{k\alpha}(\omega) V_{k\alpha} G^{R/A}_{0,0}(\omega) V_{k'\alpha'} g^{R/A}_{k'\alpha'}(\omega). & (5.87) \end{aligned}$$

Now we can look at the long-time limit of the current. From the equation for the current we see that we need to calculate $\lim_{t\to\infty} G(\xi, t)$. We will use the Riemann-Lebesgue Lemma which states that, let $f : \mathcal{R} \to \mathbb{C}$ measurable function. If $f \in \mathrm{L}^1 \Rightarrow \int_{-\infty}^{\infty} f(x) e^{-i\eta x} \mathrm{d}x \to 0$ as $\eta \to \pm\infty$.

We will make use of the following limits

$$\begin{aligned} \lim_{t\to\infty} G^{R}_{0,0}(t,0) &= \lim_{t\to\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G^{R}_{0,0}(\omega)\\ &= \lim_{t\to\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \tilde{\varepsilon}_0 - \Sigma^R(\omega) + i\eta} = 0. & (5.88)\\ \lim_{t\to\infty} \sum_k G^{A}_{0,k\alpha}(t,0) V_{k\alpha} &= \lim_{t\to\infty} \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G^{A}_{0,0}(\omega) V_{k\alpha} g^{A}_{k\alpha}(\omega) V_{k\alpha}\\ &= \lim_{t\to\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\Sigma^A(\omega) e^{-i\omega t}}{\omega - \tilde{\varepsilon}_0 - \Sigma^A(\omega) - i\eta} = 0. & (5.89) \end{aligned}$$

and

$$\begin{aligned} \lim_{t\to\infty} G^{R}_{0,k\alpha}(t,0) &= \lim_{t\to\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G^{R}_{0,k\alpha}(\omega)\\ &= \lim_{t\to\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \tilde{\varepsilon}_0 - \Sigma^R(\omega) + i\eta} \frac{V_{k\alpha}}{\omega - \tilde{\varepsilon}_{k\alpha} + i\eta}\\ &= \lim_{t\to\infty} [-iV_{k\alpha} e^{-i\tilde{\varepsilon}_{k\alpha} t} G^{R}_{0,0}(\tilde{\varepsilon}_{k\alpha})]. & (5.90)\\ \lim_{t\to\infty} \sum_k G^{A}_{k'\alpha',k\alpha}(0,t) V_{k\alpha} &= \lim_{t\to\infty} \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G^{A}_{k'\alpha',k\alpha}(\omega) V_{k\alpha}\\ &= \lim_{t\to\infty} \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} [\delta_{k'\alpha',k\alpha} g^{A}_{k'\alpha'}(\omega)\\ &\quad + g^{A}_{k'\alpha'}(\omega) V_{k'\alpha'} G^{A}_{0,0}(\omega) V_{k\alpha} g^{A}_{k\alpha}(\omega)] V_{k\alpha}\\ &= \lim_{t\to\infty} iV_{k'\alpha'} e^{i\varepsilon_{k'\alpha'} t} [\delta_{\alpha,\alpha'} + G^{A}_{0,0}(\tilde{\varepsilon}_{k'\alpha'}) \Sigma^{A}_{\alpha}(\tilde{\varepsilon}_{k'\alpha'})]. & (5.91) \end{aligned}$$

Now we can take a look at limit of the kernel $Q(\xi,t)$:

$$\begin{aligned}\lim_{t\to\infty} Q(\xi,t) &= \lim_{t\to\infty}[\boldsymbol{G}^R(t,0)\boldsymbol{G}(\xi)\boldsymbol{G}^A(0,t)]_{0,k\alpha}V_{k\alpha}\\ &= \lim_{t\to\infty}\Bigg[\sum_k G^R_{0,0}(t,0)G_{0,0}(\xi)G^A_{0,k\alpha}(0,t)V_{k\alpha}\\ &\quad+\sum_{k,k'\alpha'} G^R_{0,0}(t,0)G_{0,k'\alpha'}(\xi)G^A_{k'\alpha',k\alpha}(0,t)V_{k\alpha}\\ &\quad+\sum_{k,k'\alpha'} G^R_{0,k'\alpha'}(t,0)G_{k'\alpha',0}(\xi)G^A_{0,k\alpha}(0,t)V_{k\alpha}\\ &\quad+\sum_{k,k'\alpha',k''\alpha''} G^R_{0,k'\alpha'}(t,0)G_{k'\alpha',k''\alpha''}(\xi)G^A_{k''\alpha'',k\alpha}(0,t)V_{k\alpha}\Bigg] \qquad (5.92)\end{aligned}$$

$$\begin{aligned}&= \lim_{t\to\infty}\sum_{kk'\alpha'} G^R_{0,k'\alpha'}(t,0)\frac{1}{\xi-\tilde\varepsilon_{k'\alpha'}}G^A_{k'\alpha',k\alpha}(0,t)V_{k\alpha}\\ &\quad+\lim_{t\to\infty}\sum_{kk'\alpha'k''\alpha''} G^R_{0,k'\alpha'}(t,0)\frac{V^2_{k'\alpha'}}{\xi-\tilde\varepsilon_{k'\alpha'}}\frac{V^2_{k''\alpha''}}{\xi-\tilde\varepsilon_{k'''\alpha''}}G_{0,0}(\xi)G^A_{k''\alpha'',l\alpha}(0,t)V_{k\alpha}\\ &= \sum_{k'} G^R_{0,0}(\tilde\varepsilon_{k'\alpha})\frac{V^2_{k'\alpha}}{\xi-\tilde\varepsilon_{k'\alpha}}+\sum_{k'\alpha'} G^R_{0,0}(\tilde\varepsilon_{k'\alpha'})\frac{V^2_{k'\alpha'}}{\xi-\tilde\varepsilon_{k'\alpha'}}G^A_{0,0}(\tilde\varepsilon_{k'\alpha'})\Sigma^A_\alpha(\tilde\varepsilon_{k'\alpha'})\\ &\quad+\lim_{t\to\infty}\sum_{kk'\alpha'k''} e^{-i\tilde\varepsilon_{k'\alpha'}t}G^R_{0,0}(\tilde\varepsilon_{k'\alpha'})\frac{V^2_{k'\alpha'}}{\xi-\tilde\varepsilon_{k'\alpha'}}\frac{V^2_{k''\alpha}}{\xi-\tilde\varepsilon_{k'''\alpha}}G_{0,0}(\xi)e^{i\tilde\varepsilon_{k''\alpha}t}\\ &\quad+\lim_{t\to\infty}\sum_{kk'\alpha'k''\alpha''} e^{-i\tilde\varepsilon_{k'\alpha'}t}G^R_{0,0}(\tilde\varepsilon_{k'\alpha'})\frac{V^2_{k'\alpha'}}{\xi-\tilde\varepsilon_{k'\alpha'}}\frac{V^2_{k''\alpha''}}{\xi-\tilde\varepsilon_{k'''\alpha''}}G_{0,0}(\xi)G^A_{0,0}(\tilde\varepsilon_{k''\alpha''})\Sigma^A_\alpha(\tilde\varepsilon_{k''\alpha''})^A e^{i\tilde\varepsilon_{k''\alpha''}}.\end{aligned} \qquad (5.93)$$

Introducing the line-widht function as

$$\Gamma_\alpha(\varepsilon) = -2\mathrm{Im}[\Sigma^R_\alpha(\varepsilon)] = 2\pi\sum_k \delta(\varepsilon-\tilde\varepsilon_{k\alpha})V^2_{k\alpha} \qquad (5.94)$$

we can rewrite the limit for the kernel $Q(\xi,t)$ as

$$\begin{aligned}\lim_{t\to\infty} Q_\alpha(\xi,t) &= \int\frac{d\varepsilon}{2\pi}\frac{\Gamma_\alpha(\varepsilon)}{\xi-\varepsilon+U_\alpha}G^R_{0,0}(\xi)+\sum_{\alpha'}\int\frac{d\varepsilon}{2\pi}\frac{\Gamma_{\alpha'}(\varepsilon)}{\xi-\varepsilon+U_{\alpha'}}|G^R_{0,0}(\xi)|^2\Sigma^A_{\alpha'}(\varepsilon)\\ &\quad++\lim_{t\to\infty}G_{0,0}(\xi)\int\frac{d\varepsilon}{2\pi}\Gamma_\alpha(\varepsilon)\frac{e^{i\varepsilon t}}{\xi-\varepsilon+U_\alpha}\sum_{\alpha'}\int\frac{d\varepsilon'}{2\pi}\Gamma_{\alpha'}(\varepsilon')\frac{e^{-i\varepsilon' t}}{\xi-\varepsilon'+U_{\alpha'}}G^R_{0,0}(\varepsilon')\\ &\quad+\lim_{t\to\infty}G_{0,0}(\xi)\sum_{\alpha'}\int\frac{d\varepsilon}{2\pi}\Gamma_{\alpha'}(\varepsilon')G^R_{0,0}(\varepsilon')\frac{e^{-i\varepsilon' t}}{\xi-\varepsilon'+U_{\alpha'}}\\ &\quad\times\sum_{\alpha''}\int\frac{d\varepsilon''}{2\pi}\Gamma_{\alpha''}(\varepsilon'')G^A_{0,0}(\varepsilon'')\Sigma_\alpha(\varepsilon'')^A\frac{e^{i\varepsilon'' t}}{\xi-\varepsilon''+U_{\alpha''}}.\end{aligned} \qquad (5.95)$$

The last two terms will disappear according to Riemann-Lebesgue lemma. Finally we get an expression for the steady-state current.

$$I_R^S = -e \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_L(\varepsilon)\Gamma_R(\varepsilon)}{[\varepsilon - \varepsilon_0 - \lambda(\varepsilon)]^2 - [\Gamma(\varepsilon)/2]^2} [f(\varepsilon - U_L) - f(\varepsilon - U_R)], \tag{5.96}$$

where $\lambda(\varepsilon) = \mathrm{Re}[\Sigma^R(\varepsilon)]$ and $\Gamma(\varepsilon) = \sum_\alpha \Gamma_\alpha(\varepsilon)$. This equation gives us the steady-state current for a non-interacting system perturbed by a constant bias voltage, which appears on the distribution function f and on the quantities Γ and Λ.

5.3.2 Generalization of formula (5.96) to n-level system

In this section the Meir-Wingreen formula for the steady-state current for the n-level interacting system is derived. Leads are treated as non-interacting. Stefanucci has derived the steady-state Meir-Wingreen current for the non-interacting one-level case in his article *Time-dependent partition free approach to resonant tunneling systems* [10].

We are considering the system described by Hamiltonian

$$H = \sum_l \varepsilon_l \hat{c}_l^\dagger \hat{c}_l + \sum_{k\alpha} \varepsilon_{k\alpha} \hat{c}_{k\alpha}^\dagger \hat{c}_{k\alpha} + \sum_{ij,mn} w_{ij,mn} \hat{c}_i^\dagger \hat{c}_m^\dagger \hat{c}_k \hat{c}_n + \sum_{lk\alpha} V_{k\alpha,l} [\hat{c}_{k\alpha}^\dagger \hat{c}_l + \hat{c}_l^\dagger \hat{c}_{k\alpha}]. \tag{5.97}$$

The index α denotes the leads L, R. k is the energy levels in the leads and l, i, j, m, n are indexes for the central molecule . At t_0 the system is assumed to be at the thermodynamic equilibrium determined by inverse temperature β and chemical potential μ. At a some time t_1 the time-dependent perturbation

$$H_U(t) = \sum_{\alpha k} U_{\alpha k}(t) \hat{c}_{\alpha k}^\dagger \hat{c}_{\alpha k} + \sum_l U_l(t) \hat{c}_l^\dagger \hat{c}_l \tag{5.98}$$

is switched on.

Applying a time-dependent bias causes the single-particle energies to become time dependent $\varepsilon \to \varepsilon(t) = \varepsilon + U(t)$. The application of the bias does not change the occupation of the particular channel since the occupation is determined by an equilibrium distribution function established in the distant past.

Using the Hamiltonian (5.97) one can derive the equation of motion for the Green function

$$\left[i\frac{d}{dz}\mathbf{1} - H(z) \right] \mathbf{G}(z, z') = \delta(z, z')\mathbf{1} + \int_\gamma d\bar{z} \mathbf{\Sigma}(z, \bar{z}) \mathbf{G}(\bar{z}, z), \tag{5.99}$$

where

$$H(z) = \begin{pmatrix} E_{LL} & V_{LC} & 0 \\ V_{CL} & E_{CC} & V_{CR} \\ 0 & V_{RC} & E_{RR} \end{pmatrix} \tag{5.100}$$

is the Hamiltonian matrix describing the central system, leads and the hopping between leads and the central system.

In the chapter 3 the formula for current was derived Eq. (3.16) ($I_\alpha(z) = 2\mathrm{ReTr}\left[\mathbf{G}^<_{\alpha C}(z,z)H_{\alpha C}\right]$) The lesser Green function can be rewritten by using following formula (see Appendix G)

$$\mathbf{G}^{\gtrless}(z,z') = \mathbf{G}^R(z,0)\mathbf{G}^{\gtrless}(0,0)\mathbf{G}^A(0,z') + \mathbf{\Delta}^{\gtrless}(z,z') \tag{5.101}$$

where ($\mathbf{G}^K \equiv \mathbf{G}^> + \mathbf{G}^<$)

$$\begin{aligned}\mathbf{\Delta}^{\gtrless}(z,z') = i\mathbf{G}^R(z,0)\mathbf{G}^>(0,z') - i\mathbf{G}^<(z,0)\mathbf{G}^A(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^K(0,0)\mathbf{G}^A(0,z') \\ + \left[\mathbf{G}^R\cdot\left[\mathbf{\Sigma}^{\gtrless} + \mathbf{\Sigma}^{\rceil} * G * \mathbf{\Sigma}^{\lceil}\right]\cdot\mathbf{G}^A\right](z,z')\end{aligned} \tag{5.102}$$

If it is assumed that the Green functions vanish when the separation of their arguments goes to infinity, the expression for the greater/lesser Green function approaches following limit

$$\lim_{z,z'\to\infty}\mathbf{G}^{\gtrless}(z,z') = \mathbf{G}^R(z,0)\mathbf{\Sigma}^{\gtrless}(0,0)\mathbf{G}^A(0,z') \tag{5.103}$$

Let us look first a step-like modulation where the external perturbation is suddenly switched on, $H_U(t) = \theta(t)U_0$. Projecting the equation of motion for Green function onto the central region and solving obtained equations with help of unconnected Green functions gives us following set of equations.

$$\mathbf{G}^R_{\alpha C}(z,0) = \int d\bar{z}V_{\alpha C}\mathbf{g}^R_{\alpha\alpha}(z,\bar{z})\mathbf{G}^R_{CC}(\bar{z},0) \tag{5.104}$$

$$\begin{aligned}\mathbf{G}^R_{CC}(z,0) = \mathbf{g}^R_{CC}(z,0) + \int d\bar{z}V_{\alpha,C}\mathbf{g}^R_{CC}(z,\bar{z})\mathbf{G}^R_{\alpha C}(\bar{z},0) \\ + \int d\bar{z}d\bar{\bar{z}}\mathbf{g}^R_{CC}(z,\bar{z})\mathbf{\Sigma}_{CC}(\bar{z},\bar{\bar{z}})\mathbf{G}^R_{CC}(\bar{\bar{z}},0)\end{aligned} \tag{5.105}$$

We can also project the EOM onto the $\alpha\alpha$-region and solving the projected equations gives

$$\mathbf{G}^R_{\alpha\alpha}(z,0) = \mathbf{g}^R_{\alpha\alpha}(z,0)\delta_{\alpha\alpha'} + \int d\bar{z}V_{\alpha C}\mathbf{g}^R_{\alpha\alpha}(z,\bar{z})\mathbf{G}^R_{C\alpha}(\bar{z},0) \tag{5.106}$$

$$\mathbf{G}^R_{C\alpha}(z,0) = \int d\bar{z}V_{C\alpha}\mathbf{g}^R_{\alpha\alpha}(z,\bar{z})\mathbf{G}^R_{\alpha\alpha}(z,0) \tag{5.107}$$

Assuming that in the long time limit the Green function does not depends only on the difference of the time arguments $z - z'$ we can Fourier transform the Green function

$$\mathbf{G}(z,z') = \int\frac{d\omega}{2\pi}e^{-i\omega(z-z')}\mathbf{G}(\omega) \tag{5.108}$$

Then we can solve the central Green function in terms of the uncontacted Green function $\mathbf{g}_C$ and self-energies.

$$\mathbf{G}^R_{CC} = \frac{1}{\omega - E_c - \mathbf{\Sigma}_{em}(\omega) - \mathbf{\Sigma}(\omega) - i\eta} \tag{5.109}$$

Another later useful relation is obtained solving $\mathbf{G}_{\alpha\alpha'}$ in terms of the central Green function $\mathbf{G}_{CC}$

$$\mathbf{G}_{\alpha,\alpha'}(\omega) = \delta_{\alpha,\alpha'}\mathbf{g}_\alpha(\omega) + \mathbf{g}_\alpha(\omega)H_{\alpha C}H_{C\alpha'}\mathbf{g}_{\alpha'}(\omega)\mathbf{G}_{CC}(\omega) \tag{5.110}$$

Next let us take a look at the expression for the current. Substituting Eq. (5.101) to the current equation Eq. (3.16). Using the formula for $\mathbf{\Delta}^<(1,2)$ and recalling the definition for $\mathbf{G}^K$ we get

$$\begin{aligned} I_\alpha(t) = 2e\mathrm{ReTr}\big\{\big[&i\mathbf{G}^R(t,0)\mathbf{G}^>(0,t) - i\mathbf{G}^<(t,0)\mathbf{G}^A(0,t) - \mathbf{G}^R(t,0)\mathbf{G}^>(0,0)\mathbf{G}^<(0,t) \\ &+ \left[\mathbf{G}^R\cdot\left[\mathbf{\Sigma}^{\gtrless} + \mathbf{\Sigma}^\urcorner * G * \mathbf{\Sigma}^\ulcorner\right]\cdot\mathbf{G}^A\right](t,t)\big]_{\alpha C}H_{C\alpha}\big\} \end{aligned} \tag{5.111}$$

In the limit $t\to\infty$ the first two terms vanish since $\mathbf{G}^{\gtrless}\to 0$, when $t\to\infty$, since the separation of its time arguments goes to infinity. By looking the third term we observe that we need to find the limits for the terms $\mathbf{G}^R_{CC}(t,0)$, $\mathbf{G}^R_{C\alpha}(t,0)$ $\mathbf{G}^A_{C\alpha}(0,t)H_{\alpha C}$ and $\mathbf{G}^A_{\alpha,\alpha'}(0,t)H_{\alpha C}$

Assuming that both of the self-energies are smooth functions of ω the the integrands in the terms $\mathbf{G}^R_{CC}(t,0)$ and $\mathbf{G}^A_{C\alpha}(0,t)H_{\alpha C}$(excluding the exponential term) are absolutely convergent i.e. $\in L^1$. Because both of these functions are also measurable the Rieman-Lebesque Lemma applies giving the limit $t\to\infty$ of both Green functions $\mathbf{G}^R_{CC}(t,0)$ and $\mathbf{G}^A_{C\alpha}(0,t)H_{\alpha C}$ being equal to zero.

Next take look at the term $\mathbf{G}^R_{C\alpha}(t,0)$. Performing the Fourier-transform and using the equation $\mathbf{G}^R_{C\alpha}(\omega) = \mathbf{g}^R_\alpha(\omega)V_{C\alpha}\mathbf{G}^R_{CC}(\alpha)$ we obtain

$$\lim_{t\to\infty}\mathbf{G}^R_{C\alpha}(t,0) = \lim_{t\to\infty}\left[-ie^{-iE_\alpha t}V_{\alpha C}\mathbf{G}^R_{CC}(E_\alpha)\right] \tag{5.112}$$

Similarly the long-time limit for the term $\mathbf{G}^A_{\alpha\alpha'}(0,t)H_{\alpha C}$ is found to be

$$\lim_{t\to\infty}\mathbf{G}^A_{\alpha\alpha'}(0,t)H_{\alpha C} = \lim_{t\to\infty}\left[iV_{C\alpha}e^{-iE_\alpha t}[\delta_{\alpha\alpha'} + \mathbf{\Sigma}^A_{\alpha,em}(E_\alpha)\mathbf{G}^A_{CC}(E_\alpha)]\right] \tag{5.113}$$

The contribution to the current from the third term is then

$$\int\frac{dE}{2\pi}\left[\Gamma_\alpha(E)\mathbf{g}^>_\alpha(0)\mathbf{G}^R_{cc}(E_\alpha) + \Gamma_{\alpha'}|\mathbf{G}^R_{cc}(E_{\alpha'})|^2\mathbf{g}^>_{\alpha'}(0)\mathbf{\Sigma}^A_{\alpha,em}(E_\alpha)\right] \tag{5.114}$$

where $\Gamma(E) = 2\pi V_{C\alpha}V_{\alpha C}\delta(E-E_\alpha)$.

Taking the long-time limit in the last term we obtain

$$\lim_{t\to\infty}\left[\mathbf{G}^R\cdot\left[\mathbf{\Sigma}^{\gtrless} + \mathbf{\Sigma}^\urcorner * G * \mathbf{\Sigma}^\ulcorner\right]\cdot\mathbf{G}^A\right](t,t) = \lim_{t\to\infty}\left[\mathbf{G}^R_{cc}\cdot\mathbf{\Sigma}^<_{cc}\cdot\mathbf{G}^A_{c\alpha}\right]. \tag{5.115}$$

Fourier-transforming also this quantity gives

$$\left[\mathbf{G}^R_{cc}\cdot\mathbf{\Sigma}^<_{cc}\cdot\mathbf{G}^A_{c\alpha}\right]V_{\alpha c}=\int\frac{dE}{2\pi}\Gamma_\alpha(E)\mathbf{\Sigma}^<_{cc}(E_\alpha)|\mathbf{G}^R_{cc}(E_\alpha)|^2. \tag{5.116}$$

Combining all the terms we get a following expression for the steady-state current

$$\begin{aligned}I_\alpha=-\int\frac{dE}{2\pi}\left[\Gamma_\alpha(E)\mathbf{g}^>_\alpha(0)\mathbf{G}^R_{cc}(E_\alpha)+\Gamma_{\alpha'}|\mathbf{G}^R_{cc}(E_{\alpha'})|^2\mathbf{g}^>_{\alpha'}(0)\mathbf{\Sigma}^A_{\alpha,em}(E_\alpha)\right]\\+\int\frac{dE}{2\pi}\Gamma_\alpha(E)\mathbf{\Sigma}^<_{cc}(E_\alpha)|\mathbf{G}^R_{cc}(E_\alpha)|^2\end{aligned} \tag{5.117}$$

Finally substituting the expression for the greater lead Green function at $t=0$ ($\mathbf{g}^>_\alpha(0)=f(\varepsilon_\alpha)-1$) we found a following form for the steady-state current

$$\begin{aligned}I_\alpha=\int\frac{dE}{2\pi}\left[\Gamma_\alpha(E)\mathbf{G}^R_{cc}(E_\alpha)+\Gamma_{\alpha'}|\mathbf{G}^R_{cc}(E_{\alpha'})|^2\mathbf{\Sigma}^A_{\alpha,em}(E_\alpha)\right]\\-\int\frac{dE}{2\pi}\left[\Gamma_\alpha(E)f(E_\alpha)\mathbf{G}^R_{cc}(E_\alpha)+\Gamma_{\alpha'}|\mathbf{G}^R_{cc}(E_{\alpha'})|^2f(E_{\alpha'})\mathbf{\Sigma}^A_{\alpha,em}(E_\alpha)\right]\\+\int\frac{dE}{2\pi}\Gamma_\alpha(E)\mathbf{\Sigma}^<_{cc}(E_\alpha)|\mathbf{G}^R_{cc}(E_\alpha)|^2\end{aligned} \tag{5.118}$$

which looks a little bit different than equation (5.18). So there is mistake or several mistakes somewhere.

6 Propagation of the Green function

Our transport problem is an interacting many-particle quantum statistical problem, which can be solved using Keldysh Green function technique, where the equilibrium (Matsubara) Green function is solved first in the imaginary track and then analytically continuated to the real axis. In this chapter the propagation scheme of the Green function is shortly explained. Implementation of this scheme was mainly done by Nils Erik Dahlen.

The Hamiltonian in the site basis reads

$$\begin{aligned}\hat{\mathrm{H}}(t) = \sum_{ij\sigma} t_{ij}\hat{c}^\dagger_{j\sigma}\hat{c}_{l\sigma} + \sum_{ij,\alpha\sigma}[t_{ij\alpha} + \delta_{ij}U_\alpha(t)]\hat{d}^\dagger_{i\alpha\sigma}\hat{d}_{j\alpha\sigma} + \frac{1}{2}\sum_{ij,\sigma\sigma'} w_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{j\sigma'}\hat{c}_{i\sigma} \\ + \sum_{ij\alpha\sigma} V_{ij\alpha}[\hat{c}^\dagger_{i\sigma}\hat{d}_{j\alpha\sigma} + \hat{d}^\dagger_{j\alpha\sigma}\hat{c}_{i\sigma}]\end{aligned} \tag{6.1}$$

where the four-index dependence of the Coulomb interaction is reduced to the two-index dependence.

6.1 Kadanoff-Baym equations

The Kadanoff-Baym equations are basically the equation of motion for the different components $(\gtrless, \rceil, \lceil)$ of the Green function. These equations can be found from the basic EOM of the Green function

$$[i\partial_1\mathbf{1} - \mathbf{H}(1)]\,\mathbf{G}(1,2) = \delta(1,2)\mathbf{1} + \int_\gamma d3\mathbf{\Sigma}(1,3)\mathbf{G}(3,2) \tag{6.2}$$

and using the Langreth rules [19]. Th Kadanoff-Baym equations, which can be solved by time-propagation for the given self-energy approximation, read as

$$
\begin{aligned}
[i\partial_{t_1}\mathbf{1}-\mathbf{H}(1)]\,\mathbf{G}^{\gtrless}(1,2) &= [\mathbf{\Sigma}^R\cdot\mathbf{G}^{\gtrless}+\mathbf{\Sigma}^{\gtrless}\cdot\mathbf{G}^A+\mathbf{\Sigma}^{\rceil}\star\mathbf{G}^{\lceil}](1,2)\\
&= \mathbf{I}_1^{\gtrless}(1,2), \qquad (6.3)\\
[-i\partial_{t_2}\mathbf{1}-\mathbf{H}(2)]\,\mathbf{G}^{\gtrless}(1,2) &= \left[\mathbf{G}^R\cdot\mathbf{\Sigma}^{\gtrless}+\mathbf{G}^{\gtrless}\cdot\mathbf{\Sigma}^A+\mathbf{G}^{\rceil}\star\mathbf{\Sigma}^{\lceil}\right](1,2)\\
&= \mathbf{I}_2^{\gtrless}(1,2), \qquad (6.4)\\
[i\partial_{t_1}\mathbf{1}-\mathbf{H}(1)]\,\mathbf{G}^{\rceil}(1,2) &= \left[\mathbf{\Sigma}^R\cdot\mathbf{G}^{\rceil}+\mathbf{\Sigma}^{\rceil}\star\mathbf{G}^M\right](1,2)=\mathbf{I}^{\rceil}(1,2), \qquad (6.5)\\
[-i\partial_{t_2}\mathbf{1}-\mathbf{H}(2)]\,\mathbf{G}^{\lceil}(1,2) &= \left[\mathbf{G}^{\lceil}\cdot\mathbf{\Sigma}^A+\mathbf{G}^M\star\mathbf{\Sigma}^{\lceil}\right](1,2)=\mathbf{I}^{\lceil}(1,2), \qquad (6.6)\\
[-\partial_{\tau_1}-\mathbf{H}(1)]\,\mathbf{G}^M(1,2) &= i\delta(\tau_1-\tau_2)+\left[\mathbf{\Sigma}^M\star\mathbf{G}^M\right](1,2)\\
&= i\delta(\tau_1-\tau_2)+\mathbf{I}^M(1,2), \qquad (6.7)\\
[-\partial_{\tau_1}-\mathbf{H}(1)]\,\mathbf{G}^M(1,2) &= i\delta(\tau_1-\tau_2)+\left[\mathbf{\Sigma}^M\star\mathbf{G}^M\right](1,2)\\
&= i\delta(\tau_1-\tau_2)+\mathbf{I}^M(1,2), \qquad (6.8)
\end{aligned}
$$

where the following shorthand notation is used

$$
\mathbf{A}\cdot\mathbf{B}=\int_0^\infty \mathrm{d}t\mathbf{A}(t)\mathbf{B}(t), \qquad \mathbf{A}\star\mathbf{B}=-i\int_0^\beta \mathrm{d}\tau\,\mathbf{A}(\tau)\mathbf{B}(\tau). \qquad (6.9)
$$

The collision integrals (**I**-terms) include the history dependence and initial correlations. For example for lesser Green function

$$
\begin{aligned}
[i\partial_{t_1}\mathbf{1}-\mathbf{H}(1)]\,\mathbf{G}^{<}(1,2) = &\int_0^\infty \mathrm{d}\bar{t}\left[\mathbf{\Sigma}^R(t,\bar{t})\mathbf{G}^{<}(\bar{t},t)+\mathbf{\Sigma}^{<}(t,\bar{t})\mathbf{G}^A(\bar{t},t)\right]\\
&-i\int_0^\beta \mathrm{d}\bar{\tau}\mathbf{\Sigma}^{\rceil}(t,\bar{\tau})\mathbf{G}(\bar{\tau},t)
\end{aligned} \qquad (6.10)
$$

the real time integrals take into account the history of the system while the integration over imaginary time includes the initial correlations.

6.2 Numerical procedure

Our system is initially at equilibrium, *i.e.*, at the ground state. The system is perturbed out of the equilibrium by the applied bias voltage, which acts as an external perturbation. The numerical procedure starts from the determination of the matsubara component, the component defined in the imaginary axis, of the Green function, which describes the ground state. In other words the initial Green function will be the Hartree-Fock Green function defined on the imaginary axis. After the Green function is initialized the Dyson equation is solved on the imaginary axis, we have the interacting ground-state Green function at the HF, 2B or GW level. In the imaginary track

the Green function depends only on the difference of the time coordinates and hence it is possible to define a following simplifying notation

$$\tilde{\mathbf{G}}^M(\tau - \tau') = -i\mathbf{G}(-i\tau, -i\tau'), \tag{6.11}$$

$$\tilde{\mathbf{\Sigma}}^M(\tau - \tau') = -i\mathbf{\Sigma}(-i\tau, -i\tau'), \tag{6.12}$$

where $\tilde{\mathbf{G}}^M$ and $\tilde{\mathbf{\Sigma}}^M$ are now real quantities. The Matsubara component of the Green function is determined by solving the Dyson equation self-consistently for the equilibrium system. The imaginary time Green function solves the Dyson equation

$$[-\partial_\tau \mathbf{1} - \mathbf{h}_0]\tilde{\mathbf{G}}^M(\tau - \tau') = \delta(\tau - \tau')\mathbf{1} + \int_0^\beta \mathrm{d}\bar{\tau}\, \tilde{\mathbf{\Sigma}}(\tau - \bar{\tau})\tilde{\mathbf{G}}^M(\bar{\tau} - \tau'), \tag{6.13}$$

which can be rewritten as

$$[-\partial_\tau \mathbf{1} - \mathbf{h}_0]\tilde{\mathbf{G}}^M(\tau) = \delta(\tau)\mathbf{1} + \int_0^\beta \mathrm{d}\bar{\tau}\, \tilde{\mathbf{\Sigma}}(\tau - \bar{\tau})\tilde{\mathbf{G}}^M(\bar{\tau}). \tag{6.14}$$

By using a reference Green function G_0, the Dyson equation can be turned to following integral form

$$\tilde{\mathbf{G}}^M(\tau) = \tilde{\mathbf{G}}_0 + \int_0^\beta d\bar{\tau} d\bar{\bar{\tau}} \tilde{\mathbf{G}}_0(\tau - i\bar{\tau})\tilde{\mathbf{\Sigma}}(\bar{\tau} - \bar{\bar{\tau}})\tilde{\mathbf{G}}^M(\bar{\bar{\tau}}). \tag{6.15}$$

Because τ and τ' are in the interval $[0, \beta]$ in $\tilde{\mathbf{G}}(\tau - \tau')$ the range of τ in $\tilde{\mathbf{G}}(\tau)$ is $[-\beta, \beta]$. The Kubo-Martin-Schwinger boundary conditions for Green function and self-energy are

$$\tilde{\mathbf{G}}(\tau + \beta) = -\tilde{\mathbf{G}}(\tau), \tag{6.16}$$

$$\tilde{\mathbf{\Sigma}}(\tau + \beta) = -\tilde{\mathbf{\Sigma}}(\tau), \tag{6.17}$$

reduce the range where we need to describe functions on the half the range $[-\beta, \beta]$. This range is chosen to be $[-\beta, 0]$. The reference Hartree-Fock Green function satisfies the following equation of motion

$$\left[-\partial_\tau \mathbf{1} - \mathbf{h} - \tilde{\mathbf{\Sigma}}_0\right] \tilde{\mathbf{G}}_0(\tau) = \delta(\tau)\mathbf{1}, \tag{6.18}$$

where $\tilde{\mathbf{\Sigma}}_0(\mathbf{r}, \mathbf{r}'; \tau) = \delta(\tau)\tilde{\mathbf{\Sigma}}_0(\mathbf{r}, \mathbf{r}')$. Choosing the molecular orbitals ϕ_i such that [21]

$$h(\mathbf{r})\phi_i(\mathbf{r}) + \int \mathrm{d}\mathbf{r}' \tilde{\Sigma}_0(\mathbf{r}, \mathbf{r}')\phi_i(\mathbf{r}') = \varepsilon_i \phi_i(\mathbf{r}), \tag{6.19}$$

the $\tilde{G}^0_{ij}$ is then found to be

$$\tilde{G}^0_{ij}(\tau) = \delta_{ij}(n_i - 1)e^{-(\varepsilon_i - \mu)\tau}\theta(\tau) + \delta_{ij} n_i e^{-(\varepsilon_i - \mu)\tau}\theta(-\tau), \tag{6.20}$$

where $n_i = (e^{\beta(\varepsilon_i-\mu)}+1)^{-1}$. The reference Green function in the range $[0,-\beta]$ in the molecular orbital basis is then

$$\tilde{G}^0_{ij} = \delta_{ij}\frac{e^{\tau(\varepsilon_i-\mu)}}{e^{\tau(\varepsilon_i-\mu)}-1} \tag{6.21}$$

which is anti-periodic $\tilde{G}_0(\tau) = -\tilde{G}_0(\tau-\beta)$.

The discretisation of the imaginary time interval is done on a so-called uniform power-mesh grid. The even spaced mesh is not practical because the Green function is peaked at the ends of this time-interval (exponential terms $e^{\tau(\varepsilon_i-\mu)}$) whereas around $\beta/2$ the Green function is acting more smoothly. Therefore it is more useful to use a grid, which is denser at the ends of the interval and contains less grid-points at the middle than uniformly distributed grid. A grid suitable for this purpose is a uniform power-mesh, which is defined by three different parameters; β, u and p. The number of grid points is $M = 2up+1$, largest grid spacing is $\Delta\tau_{max} = \beta/(4u)$ while the smallest distance between the grid points is $\Delta\tau_{min} = 0.5\beta/(2^{p-1}u)$ [22].

After the Dyson equation is solved and the equilibrium Green function is obtained it is time to start to propagate the Green function to the real time-axis. The propagation is done according to the Kadanoff-Baym equations. The KKB-equations are obtained from the equation of motion of the Green function by using Langreth rules [19]. In principle what it is reached by using Langreth rules is that the EOM is analytically continuated to the real time axis.

The matsubara component of the Green function $\tilde{\mathbf{G}}^M$ is antiperiodic if the reference Green function $\tilde{\mathbf{G}}_0$ is antiperiodic thus by using the the symmetry relations of the Green function $\left[\tilde{\mathbf{G}}^{\gtrless}(1,2)\right]^* = -\tilde{\mathbf{G}}^{\gtrless}(2,1)$ and $\tilde{G}^{>}_{ij}(t,t)-\tilde{G}^{<}_{ij}(t,t) = -i\delta_{ij}$ only $\tilde{\mathbf{G}}^{>}(1,2)$ for $t_1 > t_2$ and $\tilde{\mathbf{G}}^{<}(1,2)$ for $t_1 \leq t_2$ need to be calculated and only following KB-equations need to be solved [22]

$$[i\partial_{t_1} - \mathbf{h}(1)]\,\tilde{\mathbf{G}}^{>}(1,2) = \mathbf{I}^{>}_1(1,2) \qquad [-i\partial_{t_2} - \mathbf{h}(2)]\,\tilde{\mathbf{G}}^{<}(1,2) = \mathbf{I}^{<}_2(1,2) \tag{6.22}$$

$$[i\partial_{t_1} - \mathbf{h}(1)]\,\tilde{\mathbf{G}}^{\rceil}(1,2) = \mathbf{I}^{\rceil}(1,2) \qquad [-i\partial_{t_2} - \mathbf{h}(2)]\,\tilde{\mathbf{G}}^{\lceil}(1,2) = \mathbf{I}^{\lceil}(1,2) \tag{6.23}$$

In order to start the propagation we need to specify the initial conditions. They are given by following

$$\tilde{\mathbf{G}}^{<}(0,0) = i\tilde{\mathbf{G}}^{M}(0^-) \qquad \tilde{\mathbf{G}}^{>}(0,0) = i\tilde{\mathbf{G}}^{M}(0^+) \tag{6.24}$$

$$\tilde{\mathbf{G}}^{\rceil}(t,\tau) = i\tilde{\mathbf{G}}^{M}(-\tau) \qquad \tilde{\mathbf{G}}^{\lceil}(\tau,t) = i\tilde{\mathbf{G}}^{M}(\tau) \tag{6.25}$$

The collision integrals are possessing following symmetry relations

$$\mathbf{I}^{\gtrless}(t,t') = -\left[\mathbf{I}^{\gtrless}(t',t)\right]^{\dagger} \tag{6.26}$$

$$\mathbf{I}^{\lceil}(-i\tau,t) = \left[\mathbf{I}^{\rceil}(t,-i(\beta-\tau))\right]^{\dagger} \tag{6.27}$$

Before the propagation of Green function starts the embedding self-energy $\mathbf{\Sigma}_{em}$ is solved and the self-energy appearing in the previous equations contains both the many-body self-energy and the embedding self-energy arising from the contacts.

The time-stepping is done by writing the Green function as

$$\begin{aligned}
\tilde{\mathbf{G}}^{\gtrless}(t,t') &= \mathbf{U}(t)\tilde{\mathbf{g}}^{\gtrless}(t,t')\mathbf{U}^{\dagger}(t'), && (6.28)\\
\tilde{\mathbf{G}}^{\rceil}(t,-i\tau') &= \mathbf{U}(t)\tilde{\mathbf{g}}^{\rceil}(t,-i\tau'), && (6.29)\\
\tilde{\mathbf{G}}^{\lceil}(-i\tau,t') &= \tilde{\mathbf{g}}^{\lceil}(-i\tau,t')\mathbf{U}^{\dagger}(t') && (6.30)
\end{aligned}$$

the matrix $\mathbf{U}(t)$ satisfies the equation

$$i\partial_t \mathbf{U}(t) = \mathbf{h}_{HF}(t)\mathbf{U}(t), \tag{6.31}$$

or in the other hand $\mathbf{U}(t) = e^{-i\mathbf{h}_{HF}t}$ where $\mathbf{h}_{HF} = \mathbf{h} + \mathbf{\Sigma}_{HF}$. Using the equations of motion

$$\begin{aligned}
i\partial_t \tilde{\mathbf{g}}^{>}(t,t') &= \mathbf{U}^{\dagger}(t)\mathbf{I}_1\mathbf{U}(t') && (6.32)\\
-i\partial_t \tilde{\mathbf{g}}^{<}(t',t) &= \mathbf{U}^{\dagger}(t)\mathbf{I}_2\mathbf{U}(t'), && (6.33)\\
i\partial_t \tilde{\mathbf{g}}^{\rceil}(t,-i\tau) &= \mathbf{U}^{\dagger}(t)\mathbf{I}^{\rceil}(t,-i\tau), && (6.34)\\
-i\partial_t \tilde{\mathbf{g}}^{\rceil}(-i\tau',t) &= \mathbf{I}^{\lceil}(-i\tau,t)\mathbf{U}(t.) && (6.35)
\end{aligned}$$

With help of these equations the time-stepping can be performed [22]. Time-stepping for greater and lesser Green function is

$$\begin{aligned}
\tilde{\mathbf{g}}^{>}(T+\Delta,t') &= \mathbf{U}(\Delta)\tilde{\mathbf{g}}^{>}(T,t') - \frac{1}{\mathbf{h}_{HF}}\left(1-e^{-i\Delta\mathbf{h}_{HF}}\right)\mathbf{I}_1^{>}(t') && (6.36)\\
\tilde{\mathbf{g}}^{<}(t',T+\Delta) &= \tilde{\mathbf{g}}^{<}(t',T)\mathbf{U}^{\dagger}(\Delta) - \mathbf{I}_2^{<}(t')\frac{1}{\mathbf{h}_{HF}}\left(1-e^{-i\Delta\mathbf{h}_{HF}}\right) && (6.37)
\end{aligned}$$

Time-stepping for diagonal element:

$$\begin{aligned}
\tilde{\mathbf{g}}(T+\Delta,T+\Delta) &= \mathbf{U}(\Delta)\tilde{\mathbf{g}}^{<}(T,T)\mathbf{U}^{\dagger}(\Delta)\\
&\quad - i\mathbf{U}(\Delta)\left[\int_0^{\Delta} \mathrm{d}\bar{t}\,\mathbf{U}^{\dagger}(\bar{t})\mathbf{I}_{12}^{<}\mathbf{U}(t)\right]\mathbf{U}^{\dagger}(\Delta)\\
&= \mathbf{U}(\Delta)\left[\tilde{\mathbf{g}}^{<}(T,T) + \sum_{n=0}^{\infty} C^n\right]\mathbf{U}^{\dagger}(\Delta)
\end{aligned} \tag{6.38}$$

where $C^n = \frac{i\Delta}{n+1}[\mathbf{h}_{HF}C^{n-1}]$.

Time-stepping for the mixed terms:

$$\begin{aligned}
\tilde{\mathbf{g}}^{\lceil}(-i\tau,t'+\Delta) &= \tilde{\mathbf{g}}^{\lceil}(-i\tau,t')\mathbf{U}^{\dagger}(\Delta) - \frac{1}{\mathbf{h}_{HF}}\left(1-e^{i\Delta\mathbf{h}_{HF}}\right)\mathbf{I}^{\lceil}(-i\tau') && (6.39)\\
\tilde{\mathbf{g}}^{\rceil}(t+\Delta,-i\tau') &= \mathbf{U}(\Delta)\tilde{\mathbf{g}}^{\rceil}(t,-i\tau') - \frac{1}{\mathbf{h}_{HF}}\left(1-e^{-i\Delta\mathbf{h}_{HF}}\right)\mathbf{I}^{\rceil}(-i\tau') && (6.40)
\end{aligned}$$

Where it is assumed that the Green functions are know for times $t, t' < T$ and Δ is a small time-step. For a more detailed discussion of the numerical procedure I refer to the thesis of Karsten Balzer [22].

7 Results

In this work I studied the electron transport through molecular chains of different length modeled with tight binding approximation. The system is connected to the macroscopic one-dimensional tight-binding electrodes. The main properties being investigated were the effect of different self-energy approximations to the transient and steady-state currents and the effect of the conductivity of the central molecule to the current. All the results are presented in atomic units.

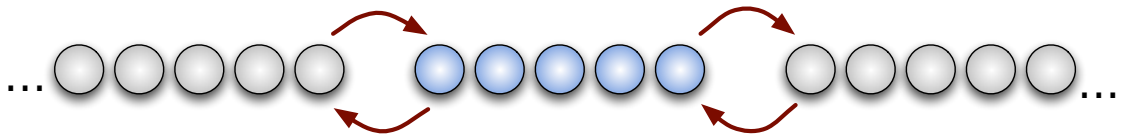

Figure 7.1: Schematic picture of the system.

The parameters characterizing the leads are tight-binding parameters a and b, which will be denoted in future simply by $\mathrm{a_{lead}}$ and $\mathrm{b_{lead}}$. These describe the on-site repulsion and the hopping probability between the sites. The $\mathrm{a_{lead}}$-parameter is taken to equal to the chemical potential resulting half-filled lead energy continuum, whereas $\mathrm{b_{lead}}{=}{-}2.0$. The central molecule has its own $\mathrm{a_{cen}}$ and $\mathrm{b_{cen}}$ parameters. In the following $\mathrm{a_{cen}}{=}0$. The strength of the coupling of the molecule to the leads is denoted by parameter V.

The electron-electron interactions in the code are reduced to depend only of two indices $w_{ijkl} = \delta_{il}\delta_{jk}v_{lj}$ where $v_{ij} = u/(2|i-j|)$ if $i \neq j$ and $v_{ii} = u$. I took $u{=}2.0$ The length of the time-step t_{step} is 0.05. The spectral functions are presented up to a normalization factor.

There are three different ways to switch on the applied bias voltage, and in addition we can also use an oscillating AC field. First bias type is sudden switch on where the bias voltage is switched at $t = t_0$ to some constant value U. The second type is sinusoidal switching where the bias follows sine to the power of two function until it reaches it maximum amplitude

$$\mathrm{U_L}(t) = \begin{cases} \mathrm{U}\sin^2(\omega t) & t < \frac{\pi}{2\omega} \\ \mathrm{U} & t > \frac{\pi}{2\omega} \end{cases} \tag{7.1}$$

and the bias of the right lead is $U_R(t) = -U_L(t)$. The third way to switch the bias on is to use error-function

$$\mathrm{U_L}(t) = \begin{cases} \mathrm{U}\mathrm{erf}(\omega t) & t < \frac{\pi}{2\omega} \\ \mathrm{U} & t > \frac{\pi}{2\omega} \end{cases} \tag{7.2}$$

and the bias of the right lead is $\mathrm{U_R(t)}$=-$\mathrm{U_L(t)}$.

The AC-bias is characterized by the following equations

$$\begin{aligned} \mathrm{U_L}(t) &= \mathrm{U}\sin(\omega t), \\ \mathrm{U_R}(t) &= -\mathrm{U}\sin(\omega t). \end{aligned} \tag{7.3}$$

7.1 One-level system

The standard example of the transport in the literature is the resonant level model, which is consisting of one level between the leads. As an example of the result given by KB-code, the current through this model is calculated with two different couplings between the leads and central region.

Although, the interacting region is consisting only of one site the current given by 2B and GW self-energy approximations differs from the current given by HF self-energy approximation. The Hartree-Fock approximation gives highest value for the steady-state current because the area under the spectral peak inside the bias window, $[1.001, 3.001]$, is largest. Also, the area inside the bias window for GW spectral peak is a little bit larger than the area inside the bias window for 2B spectral peak and, therefore, the value of the steady state current is larger with GW approximation than with the 2B approximation.

Next we loo at the IV-curves. The IV-curve of the HF approximation has the steepest slope because the area under the spectral peak inside the bias window increases most rapidly compared to the other self-energy approximations. The 2B and GW IV-curves are quite similar because their spectral functions are almost the same.

The coupling does not affect to the difference in the steady-state value of current with different self-energy approximations. The Hartree-Fock approximation gives the highest current whereas the second Born and GW approximations give smaller current. The increase of the coupling between leads and central system causes only a higher value for the steady-state current compared to its value with weaker coupling.

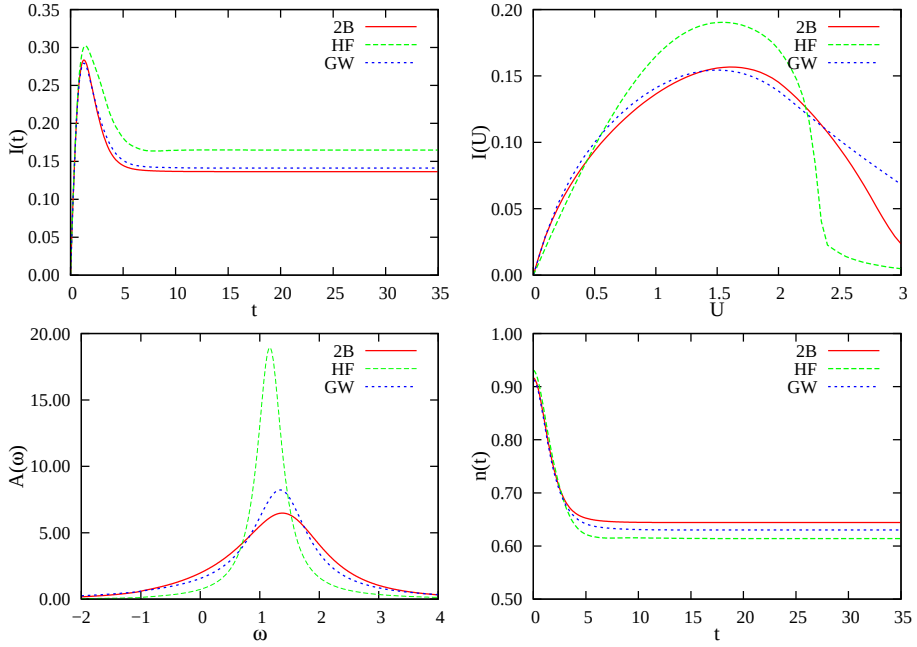

Figure 7.2: Coupling V=0.5 bias voltage U=1.0, bias type: $\sin^2$, central system hopping parameter -1.0. *Top left:* Current through the right lead. *Top right:* IV-curve. *Bottom left:* Spectral function up to a normalization factor. *Bottom right:* Site density.

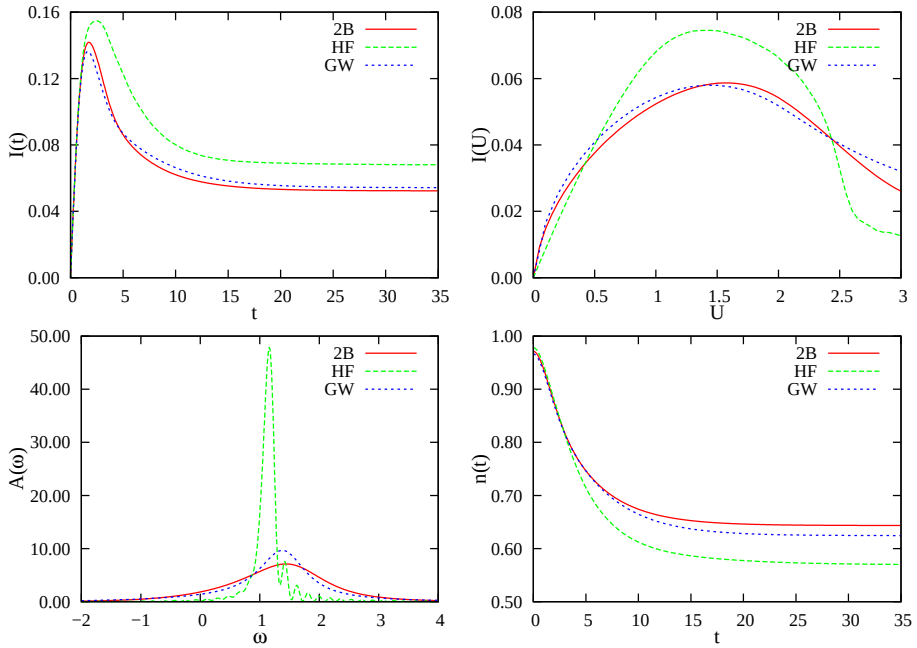

Figure 7.3: Coupling V =0.3 bias voltage $U = 1.0$, bias type: $\sin^2$, central system hopping parameter -1.0. *Top left:* Current through the right lead. *Top right:* IV-curve. *Bottom left:* Spectral function up to a normalization factor. *Bottom right:* Site density.

7.2 Two-level system

Next example is a system, which consist of two sites. This system is studied with the same method by Myöhänen *et.al* [23] where it is shown that the oscillations of the transient current and of the site densities correspond to electron transitions between the lead and the central sites. The steady-state current depends also on the memory, *i.e.*, which self-energy approximation is used. In the transient regime they show that neglecting the initial correlations produces a completely different current although the long time limits with and without initial correlations produce the same nonequilibrium steady-state current.

The purpose of the next few results is to show how the conductivity of the central region, *i.e.*, the magnitude of the tight-binding hopping parameter between the central sites affects to the site densities and to the polarization of the system. In the figure 7.4 is an example of transient currents with hopping parameters -0.3 and -0.6.

The steady-state value of the current is highest with the Hartree-Fock approximation which is because the spectral weight inside the bias window $[1, 3]$ is largest with HF compared to 2B and GW - approximations whose spectral functions are broader.

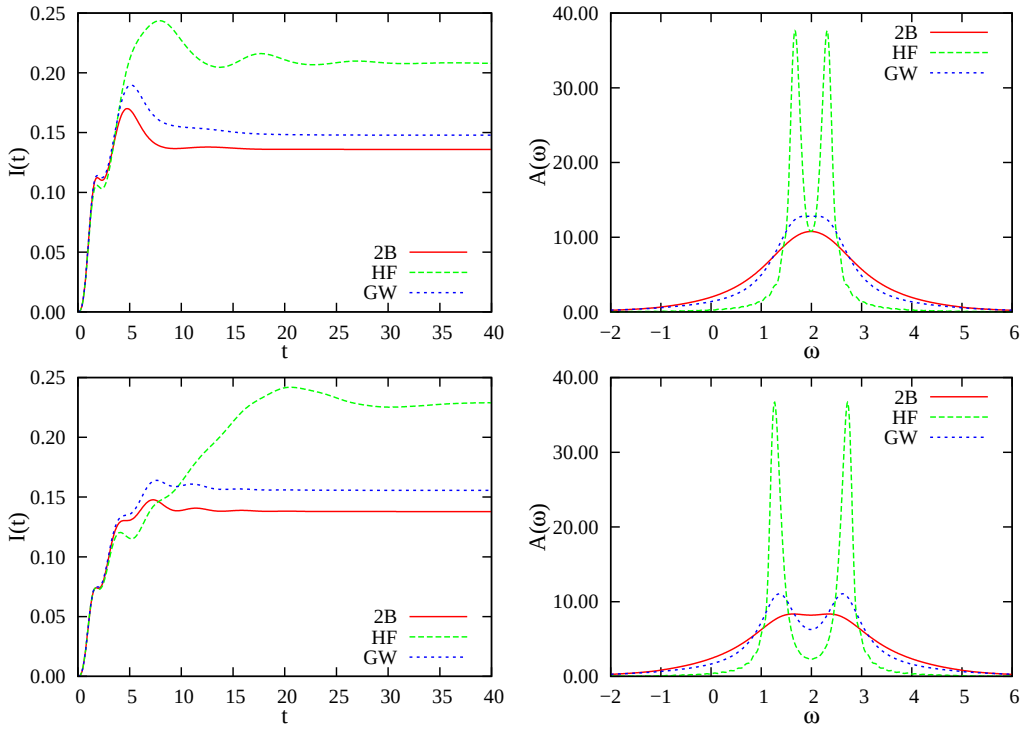

Figure 7.4: Coupling V=0.5 bias voltage U=1.0, bias type: $\sin^2$, central region hopping parameter -1.0. *Top left:* Current through the right lead. *Top right:* IV-curve. *Bottom left:* Spectral function up to a normalization factor. *Bottom right:* Site density.

In the figure 7.5 the site densities for 2B-approximation are shown with four different hopping parameter b_{cen} between the central sites $\{-0.3, -0.4, -0,5, -0.6\}$. If $|b_{cen}|$ <V, where V denotes the strength of the coupling, the density accumulates to the first site. By increasing the magnitude of the tight-binding hopping parameter, the density accumulates to the second site if $|b_{cen}|$ >V. The oscillations of the site densities are also lasting longer when the central system becomes more conductive.

With five site system the effect of hopping parameter b_{cen} between the central sites is investigated more and with more larger magnitudes of b_{cen}. Also the effect of different bias-voltages and switching of voltages is investigated.

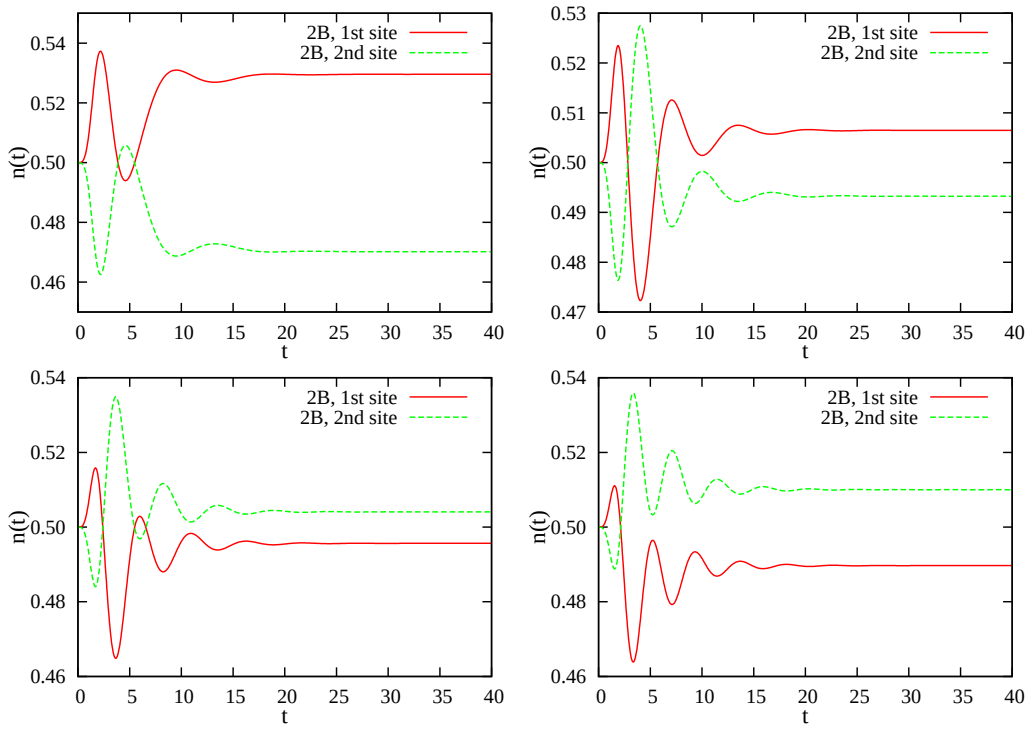

Figure 7.5: Coupling V=0.3 bias voltage U=1.0, bias type: $\sin^2$, central region hopping parameter -1.0. *Top left:* Density of the sites, $b_{cen} = -0.3$. *Top right:* Density of the sites, $b_{cen} = -0.4$. *Bottom left:* Density of the sites, $b_{cen} = -0.5$. *Bottom right:* Density of the sites, $b_{cen} = -0.6$.

7.3 Five-level system

The final system consists of five sites in the central region. The effect of different bias voltages to the steady state current is investigated. Also the effect of initial correlations and history dependence (different self-energy approximations) to the steady-state current is studied. The conductivity properties of the central region and its effects to the site densities is another topic.

The difference between the different electron self-energy approximations to the transient and steady-state current is presented on top left of the figure 7.6, where the coupling between the leads is 0.3 and amplitude of the bias is 0.8. The Hartree-Fock approximation gives a lot smaller current compared to the 2B and GW approximations. The reason for this is that in the HF spectral function the spectral weight inside the bias window ($[\mu - \mathrm{U}, \mu + \mathrm{U}] = [3.92, 5.52]$) is smaller compared to 2B and GW approximations (see top right of Fig. 7.6). In the HF-approximation the quasiparticle states are just outside of the bias window when in the 2B and GW approximations the HOMO/LUMO-states are just inside the bias window.

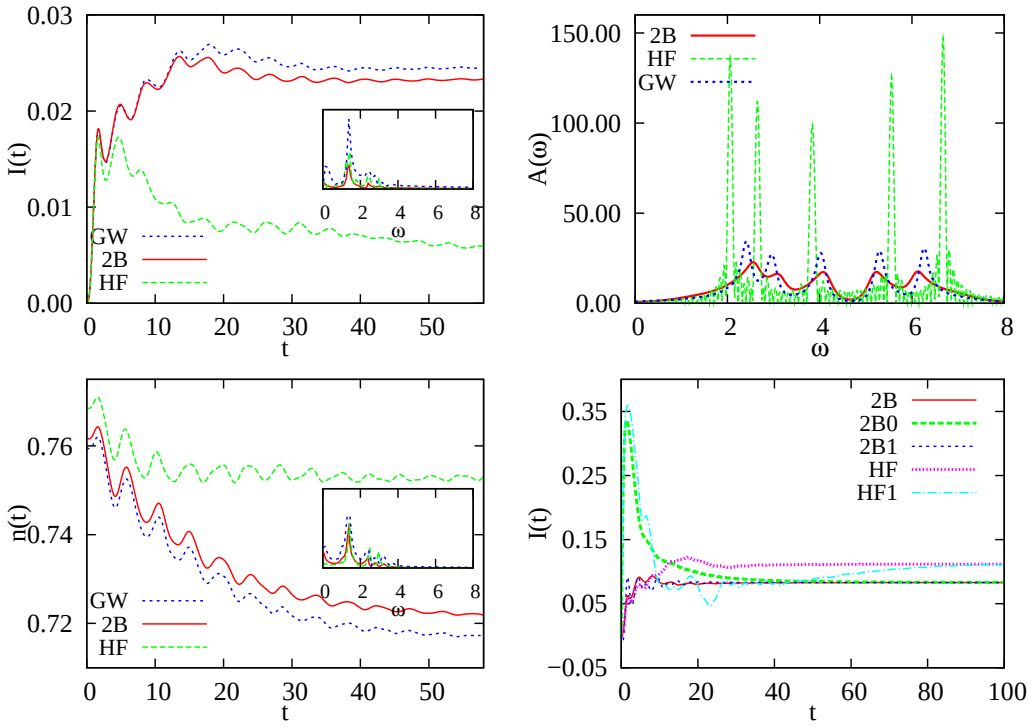

Figure 7.6: Coupling V=0.3, amplitude of the bias U=0.8, bias type $\sin^2$, ω=1.0, central-area hopping term $\mathrm{b_{cen}} = -1.0$. *Top left*: Current through right lead by using different self-energy approximations. *Top right:* Spectral functions with different self-energy approximations (up to a normalization factor). *Bottom left:* The site density of the first site with different self-energy approximations *Bottom right:* The effect of the initial correlations to the current.

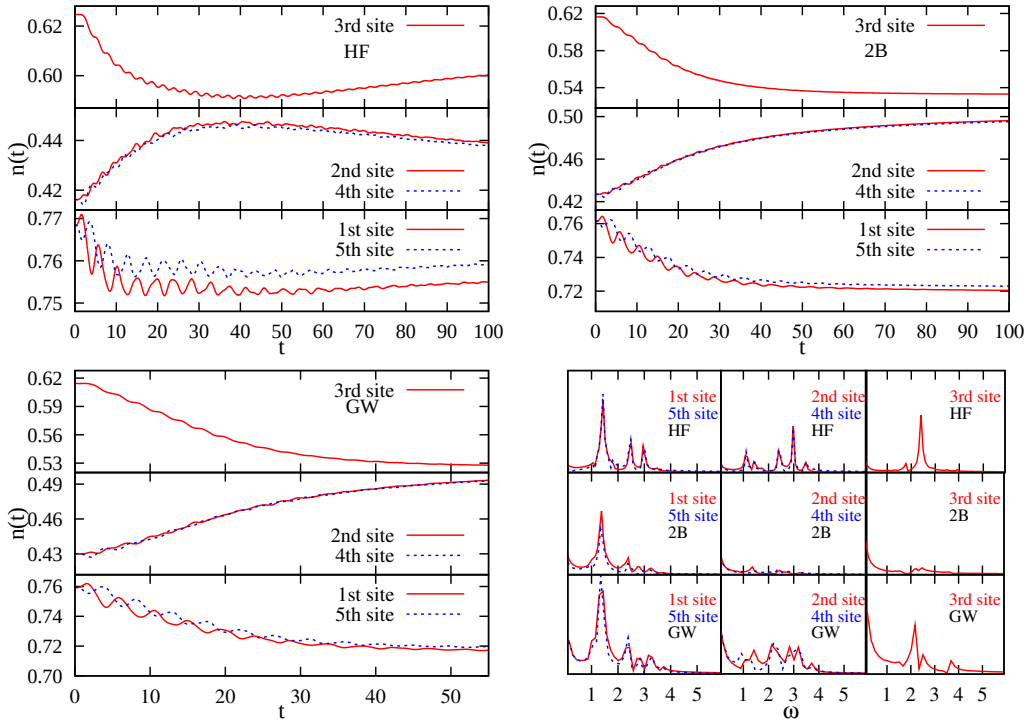

Figure 7.7: Coupling V=0.3, amplitude of the bias U=0.8, bias type $\sin^2$, ω=1.0, central system hopping term $b_{cen} = -1.0$. *Top left:* Electron density for sites one and five using Hartree-Fock approximation. *Top right:*Electron density for sites one and five using second Born approximation. *Bottom left:* Electron density for sites one and five using GW approximation. *Bottom right:* Fourier-transforms of site densities.

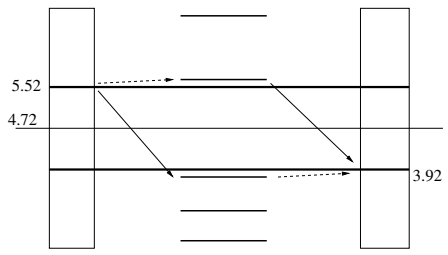

Figure 7.8: A sketch of the energy levels of the system through which the electrons propagate (HF).

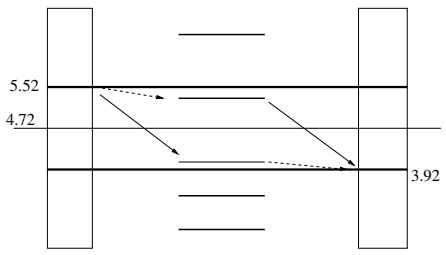

Figure 7.9: A sketch of the energy levels of the system through which the electrons propagate (2B)

The oscillations of the current are consequence of the oscillations of the site densities, the largest contribution coming from the oscillations in the first and last site (see Fig. 7.7 and the bottom left of Fig. 7.6). The frequency of the oscillations can be identified to correspond the transition of electrons from the lead to the central system and vice versa. The frequency corresponding this transition is given as

$$\omega_i^{\pm} = \varepsilon_i - \mu \pm \mathrm{U}, \tag{7.4}$$

where U is the amplitude of the applied bias voltage, μ is the chemical potential and ε is the energy of the quasi-particle state.

Chemical potential of the system is at μ=4.72, so that there is three orbitals occupied and two are unoccupied. The highest occupied state within HF approximation is at $\varepsilon^{\mathrm{HF}}_{\mathrm{HOMO}}$=3.85 and the lowest unoccupied state is at $\varepsilon^{\mathrm{HF}}_{\mathrm{LUMO}}$=5.56. Within 2B approximation the corresponding states are at $\varepsilon^{\mathrm{2B}}_{\mathrm{HOMO}}$=4.07 and $\varepsilon^{\mathrm{2B}}_{\mathrm{LUMO}}$=5.28. The highest peaks in the Fourier transforms of current occur at frequencies corresponding the transition between leads and the HOMO/LUMO-states ($\omega_1^{\mathrm{HF}} \approx 0.04$, $\omega_2^{\mathrm{HF}} \approx 1.67$ $\omega_1^{\mathrm{2B}} \approx 0.24$, $\omega_2^{\mathrm{2B}} \approx 1.45$). The oscillations of the site densities have a frequency, which also corresponds to these transitions. The possible transitions are shown in the figures 7.8 and 7.9.

The occupation of the levels at different instants of time helps us to draw conclusions of which quasiparticle states are contributing to the transmission. In this case the transmission occurs mainly through HOMO/LUMO-states. The lowest two states, which are fully occupied at the beginning, remain occupied during the propagation. The highest state, which is unoccupied at the beginning, remains practically unoccupied during the propagation. The Fourier-transform of the current supports this picture, the two highest peaks are corresponding to the transitions to/from the HOMO/LUMO-states.

The electron density does not spread uniformly between the central region sites. The density of electrons per spin is highest in the first and last sites whereas in the second and fourth sites the density is smallest. This is a consequence of the fact that electrons are trying to minimize their coulomb repulsion. Applying a bias voltage increases this difference. When the applied bias voltage is weak the difference between distinct sites is biggest. Increasing the bias voltage causes the electrons to distribute to more smoothly.

The amplitude of the site density oscillations depends on several things. Firstly they depend on the coupling between the leads and the central region. If the coupling constant is small compared to the tight-binding hopping parameter in the central area, the probability for reflection at the central-area/lead boundary is higher than transmission. The electron density is, therefore, oscillating back and forth a longer time, before it has dissipated its energy to the leads; energy which was gained when the electron has hopped from the lead to the central-region state.

By using the HF approximation the quasiparticle states are sharper and more distinct compared to 2B and GW approximations. The oscillations in the site densities are bigger when the peaks in the spectral function are sharper. For example changing the central molecule hopping parameter we can make the central molecule quasiparticle states more degenerate by decreasing the hopping parameter and by increasing a more separated.

The oscillations of the site densities increase with increasing the central molecule tight-binding hopping parameter. Decreasing the b_{cen} (increasing $|b_{cen}|$) we make the central region more conducting and the frequency of the oscillations increases. The increase of the frequency is on the other hand consequence of the fact the HOMO/LUMO-states further from the bias-window edge but also the ease for electrons to bounce back and forth could increase the frequency of the oscillations.

When the value of b_{cen} is small the central-area states come closer together and with second Born and GW-approximations it is not possible to talk of distinct states any more. Analysing the occupation of the orbital-states and comparing the frequencies obtained from the Fourier-transforms of the current and site-densities, it is seen that all of the orbitals are involved in the transmission. In Hartree-Fock approximation only the HOMO/LUMO-states are involved in the transport of electrons. If $b_{cen}=-1.0$ or larger only the HOMO/LUMO-states are used in the transport with all of the self-energy approximations.

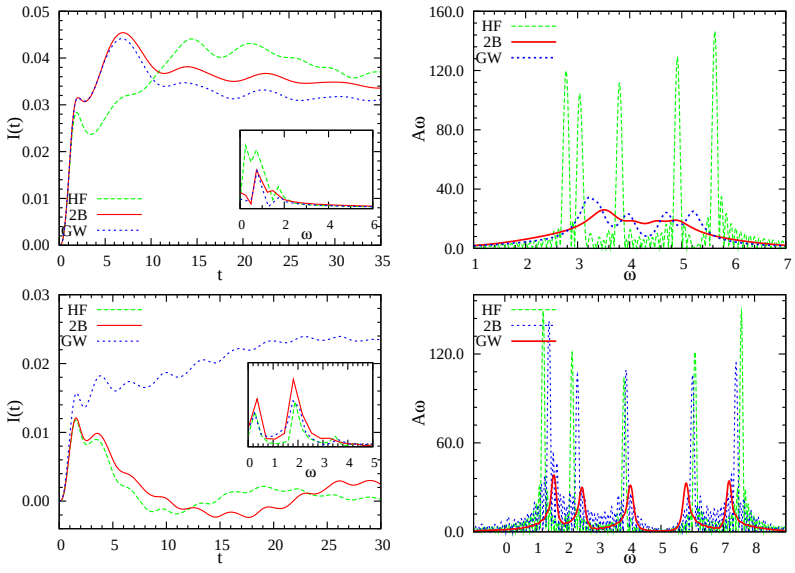

Figure 7.10: Coupling V=0.3, amplitude of the bias U=0.8, bias type $\sin^2$, ω=1.0. *Left up:* Current through the system, $b_{cen}=-0.5$. In the inset is Fourier-transform of the current. *Right up:* Spectral functions up to a normalization factor, $b_{cen}=-0.5$. *Left down:* Current through the system, $b_{cen}=-1.5$. In the inset is Fourier-transform of the current. *Right down:* Spectral functions up to a normalization factor, $b_{cen}=-1.5$.

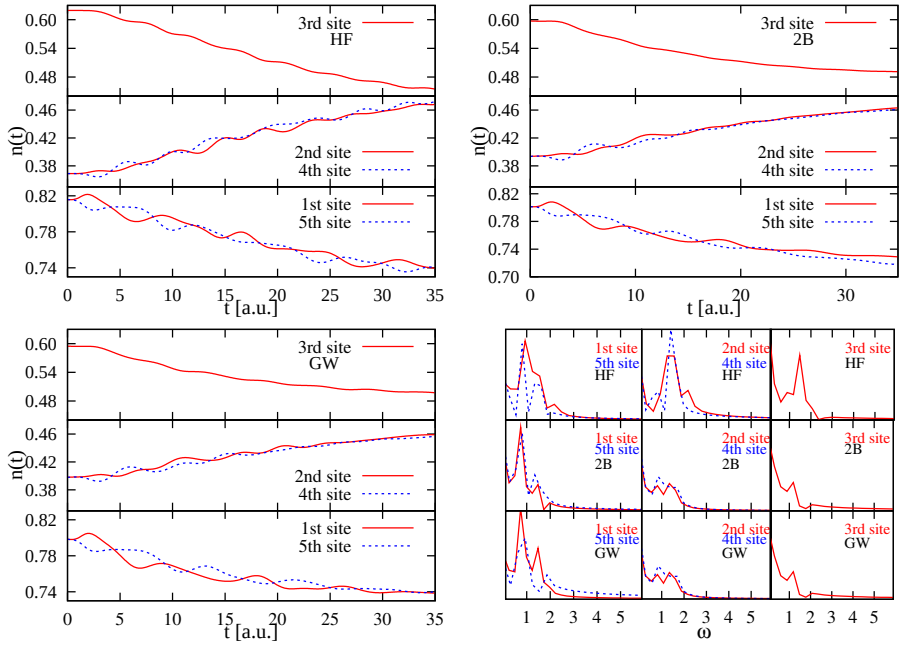

Figure 7.11: Coupling V=0.3, amplitude of the bias U=0.8, central-area hopping term $b_{cen}=-0.5$. *Top left:* Electron density for sites one and five using Hartree-Fock approximation. *Top right:*Electron density for sites one and five using second Born approximation. *Bottom left:* Electron density for sites one and five using GW approximation. *Bottom right:* Fourier-transforms of site densities.

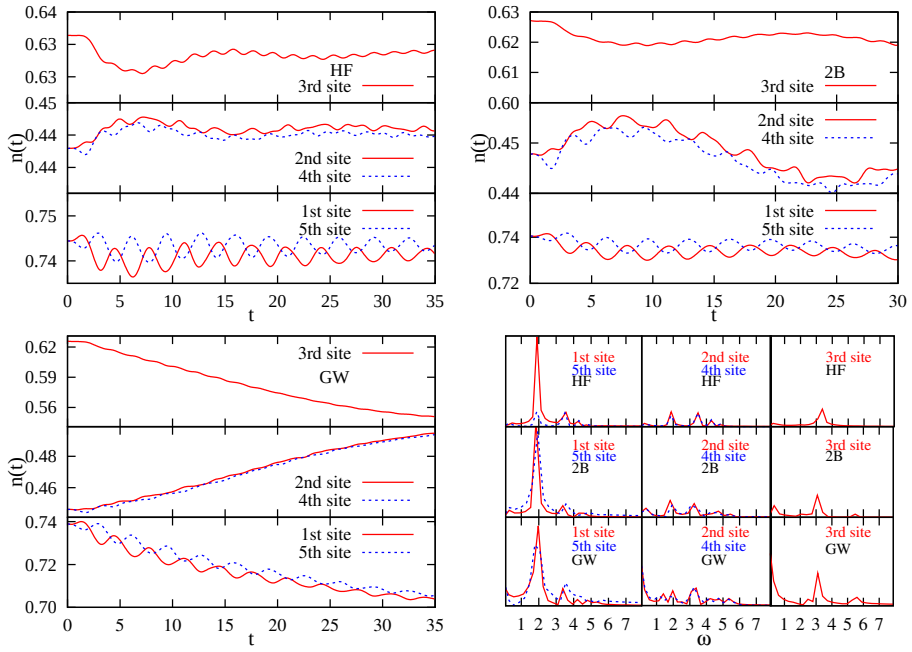

Figure 7.12: Coupling V=0.3, amplitude of the bias U=0.8, central-area hopping term $b_{cen}=-1.5$. *Top left:* Electron density for sites one and five using Hartree-Fock approximation. *Top right:*Electron density for sites one and five using second Born approximation. *Bottom left:* Electron density for sites one and five using GW approximation. *Bottom right:* Fourier-transforms of site densities.

The amplitude of the oscillations depends also on the applied bias voltage. If we have small coupling to the leads and small bias voltage the oscillations in the site densities have larger amplitude compared to the situation with larger bias voltage. This is natural since the larger potential difference between the electrodes will prefer the flow of electrons through the system while with small voltages the electrons will more likely bounce back and forth if the central region if the coupling is weak enough.

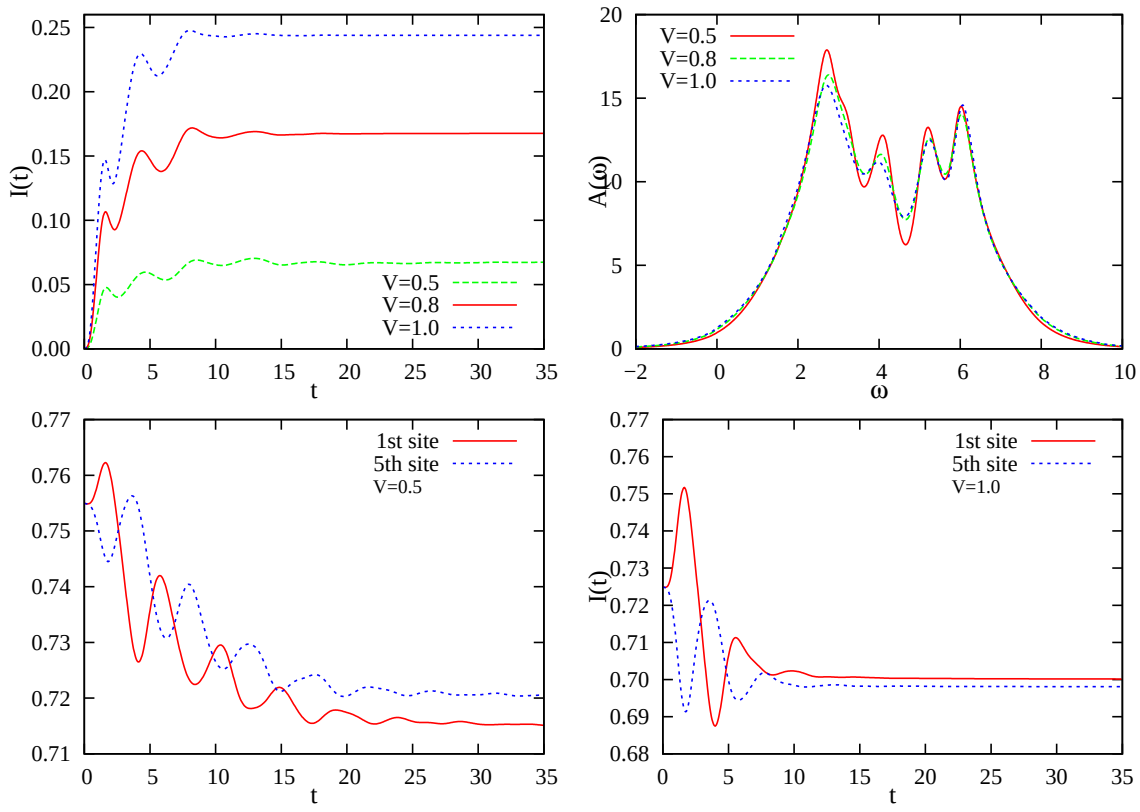

Figure 7.13: *Top left:* Current through right lead with different coupling constants using 2B approximation U=0.8, bias type $\sin^2$, ω=1.0. *Top right:* Spectral function up to a normalization factor with different coupling constants. *Bottom left:* Electron density of first and fifth sites. Coupling constant is 0.5 *Bottom right:* Electron density of first and fifth sites. Coupling constant is 1.0.

In the bottom left of the figure 7.6 the effect of the initial correlations to the current is investigated. 2B is the full second Born calculation when in the 2B0 calculation the initial correlations are excluded i.e. both the many-body and embedding the terms $\Sigma^{\lceil/\rceil}_{\mathrm{MB/em}}$ are not taken into account. In 2B1 calculation only the many-body part $\Sigma^{\lceil/\rceil}_{\mathrm{MB}}$ of the initial correlations is excluded. The same naming conventipm applies also for the Hartree-Fock approximation but in that case there is no $\Sigma^{\lceil/\rceil}_{\mathrm{MB}}$ terms. In the Hartree-Fock and second Born approximations with and without initial correlations approach same steady-state value for the current respectively. This is accordance with the memory-loss theorem, which says that the current is independent of the initial-state [10].

In Fig. 7.14 the bias voltage is applied in a different ways. First the effect of different types of switching of bias voltage to the transient current is shown in top left of the figure 7.14, where the applied bias is switched on using sudden switch-on, $\sin^2$-type and erf-type of switching. The amplitude of the voltage is 0.8 while the couplings between the leads are 0.3. The effect of type of bias voltage to the transient current is how smoothly the steady-state current develops. With all the calculated parameters the steady-state current is same regardless of the applied bias.

The type of bias affects to the overshoot effect in the transient current and after the system reaches the nonequilibrium steady state the system has forgotten how the bias was switched on. Highest overshoot effect is obtained with the sudden switching since response of the electron velocity to the abrupt change in the voltage is larger than the response of the electron energy. After energy relaxation time τ_E the system relaxates toward equilibrium. Switching on the bias more smoothly can reduce this overshoot effect. Decreasing the value of the ω parameter gives the system more time to relax and therefore the overshoot disappears.

The bias is also switched on at different times and the bias voltage is also applied using different frequency. In all these cases the steady-state currents have a same value respectively. In the inset of top right of figure 7.14 are initial and final spectral distribution for ω=1.0. The spectral distribution at the end of the propagation is more broaden and also the HOMO/LUMO-gap has decreased compared to the initial spectral distribution. In the bottom right of the Fig. 7.14 is a example of satisfaction of the continuity equation. The change of particles in the central area equals to the sum of the left and right currents.

Applying the bias voltage causes the system to become polarized; the charge density is higher at right side of the chain if the absolute value of the ratio between coupling constant and central-hopping parameter is larger than one; approximately $|b_{cen}/V| > 1$. If $|b_{cen}/V| < 1$ the density will be higher on the left side of the chain. Where the polarization of the central system changes depends also from the amplitude of the applied bias voltage. The polarization is higher if the bias voltage is small, because then he larger amplitudes of the voltage will prefer the flow of electrons through the system instead of accumulation of the density.

In figure 7.15 the density of first and fifth site is plotted for four different central system hopping parameters. For small hopping parameters the electron density accumulates to the left, while with larger hopping parameters, the density accumulates to the right.

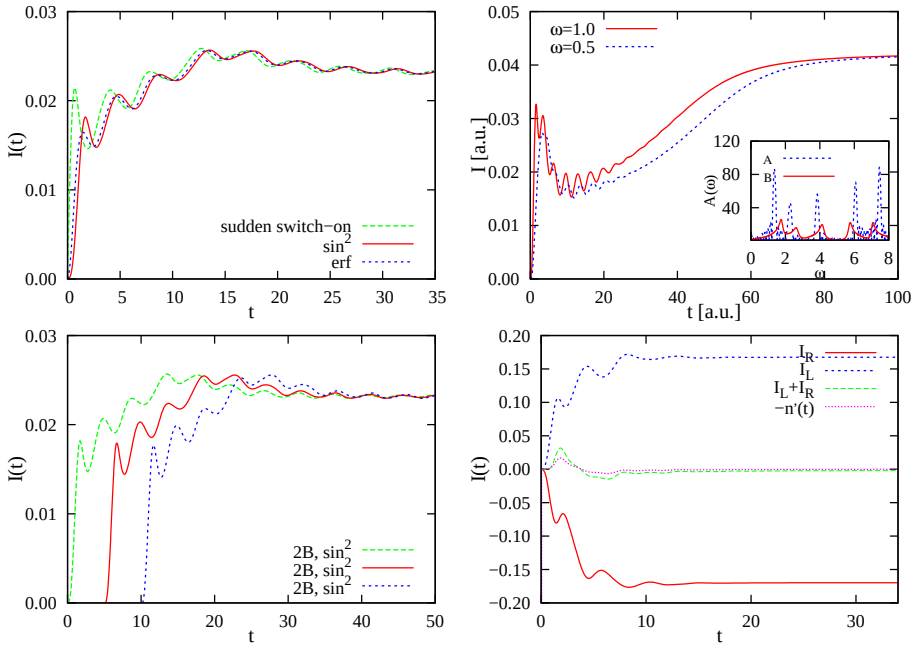

Figure 7.14: *Top left:* Different type of bias voltages with 2B-approximation. *Top right:* Switching the $\sin^2$-type of bias with different values of ω, 2B. *Bottom left:* Current through right lead, switching the bias on at different times, 2B. *Bottom right:* The validity of continuity equation.

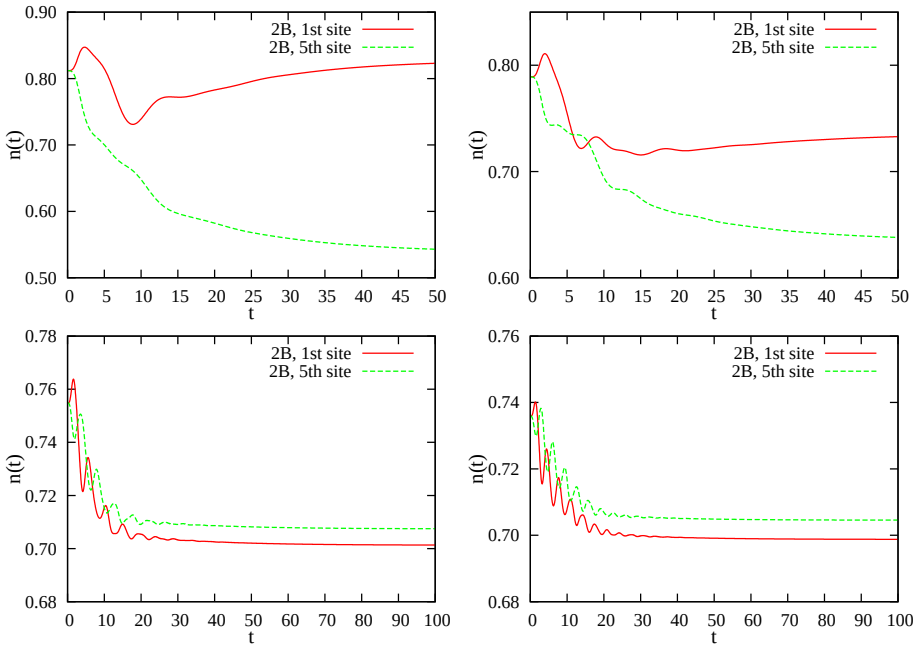

Figure 7.15: Coupling: 0.5, U=1.0, bias type: $\sin^2$ with ω=1.0. *Top left:* Density of first and fifth site, b_{cen}=0.3. *Top right:* Density of first and fifth site, b_{cen}=0.5. *Bottom left:* Density of first and fifth site, b_{cen} = 1.0. *Bottom right:* I Density of first and fifth site, b_{cen}=1.5.

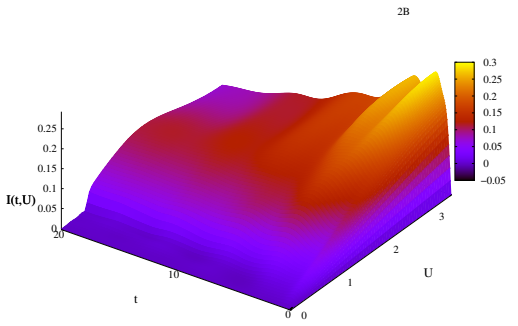

Figure 7.16: (t,U,I)-contour, second Born approximation, coupling between leads V=0.5.

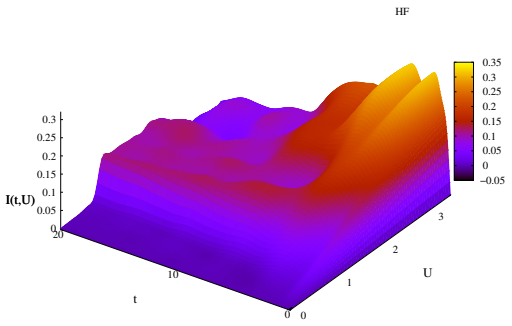

Figure 7.17: (t,U,I)-contour, Hartree-Fock approximation, coupling between leads V=0.5.

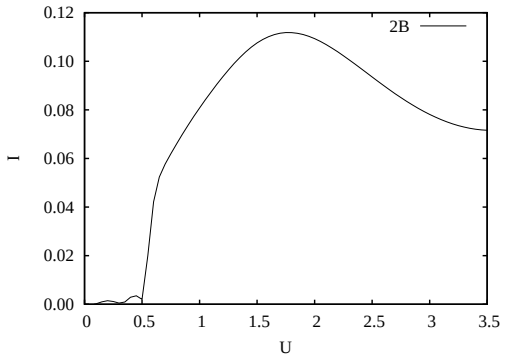

Figure 7.18: IU-curve, Second Born approximation, coupling between leads V=0.5.

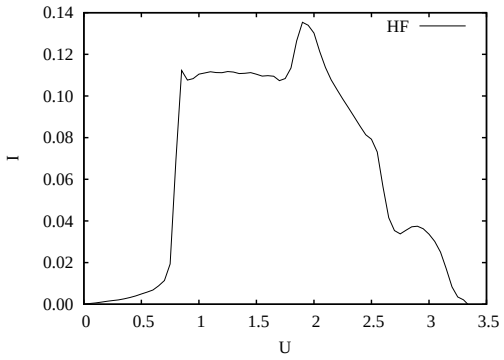

Figure 7.19: IU-curve, Hartree-Fock approximation, coupling between leads V=0.5.

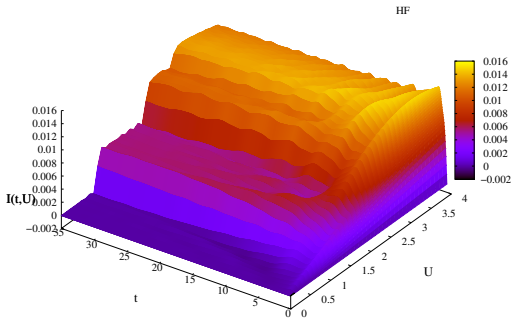

Figure 7.20: (t,U,I)-contour, Hartree-Fock approximation, coupling between leads V=0.1.

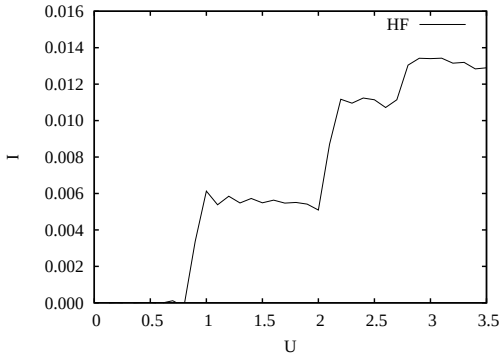

Figure 7.21: IU-curve, Hartree-Fock approximation, coupling between leads V=0.1.

Sweeping the voltage values for certain range we can make a contour plot in the (t,U,I)-space. In the Hartree-Fock approximations we can see the step-structure, the current increases step-like fashion when new quasiparticle states move into the bias window. Because in the Hartree-Fock approximation the quasiparticle state are sharper compared to second Born and GW-approximations, the steps are appearing more clearly. Especially in Fig. 7.20 where the coupling between the leads is 0.1, i.e. the central region states are perturbed as little as possible we have a very clear staircase structure.

In the figure 7.20 it is possible to see the formation of the plateaus. For example in the formation of the zero current and first plateaus around U=1 the current flows at small times but the long-time limit of the current is zero. At slightly larger voltages the long-time limit of the current goes to the first plateaus.

Taking the values of current and voltage and the end of the propagation we are able to plot the (I,U)-curves, from which the steps in the Hartree-Fock approximations are seen more clearly.

8 Summary & Outlook

The nonequilibrium Green functions and Kadanoff-Baym equations made it possible to study the time-dependent currents through an interacting quantum system. The Green function is defined as an expectation value of time-ordered product of an annihilation and creation field operator. This expectation value can be expressed on the Keldysh-contour by using the time-evolution operator. After the derivation of equation of motion for Green function and extracting the different components, we end up to the KB-equations, which include the history dependence and initial correlations.

Defining the embedding self-energy, which takes care of the leads, we turned the problem of open quantum system to a closed one. Therefore only the central system Green function is needed to be solved to obtain the current through the lead α. The equation of motion for the central system Green function includes both the many-body self-energy and the embedding self-energy. The most important thing when choosing the many-body self-energy approximation is that it has to be Φ-derivable in order to satisfy the macroscopic conservation laws.

The current in the transient regime shows oscillations, which are consequence of the oscillations of the site-densities. In addition the oscillations in the site densities turned out to be consequence of transition of the electrons from the lead to the central-area and vice versa. The steady-state value of the current depends on the history i.e. used self-energy approximation. The steady-state values for current calculated with the second Born or GW-approximations are usually close each other whereas the Hartree-Fock approximation gives sometimes higher value for the steady-state current and sometimes lower.

The system becomes polarized during the time-propagation. The electron density is accumulating to the right if approximately $|b_{cen}/V| > 1$ otherwise the density is accumulating to the left. The switching the bias different ways does not seem to affect to the steady state, at least with the calculated parameters. Neglecting initial correlations affect to the transient current but the steady-state current is same.

This same method can be improved to transport problems with two or three dimensional leads. By including more sites into the central region it is also possible to construct an interacting tips connected to the linear-chain or benzene ring. The benzene ring calculations with one-dimensional chain are one of the future tasks what one should to.

Including spin of the electron is a step forward because now we are dealing with spin-polarized systems. Including magnetic fields and studying transport under a both electric and magnetic fields is an interesting future problem. Another way to proceed is the time-dependent density functional theory and derivation of new functionals using the Green function theory, which are suitable to describe the transport problem. The currents calculated via TDDFT are also more comparable to the experimental results than KB-calculations with used basis.

Appendix A: Gell-Mann and Low theorem and adiabatic switching on

In the adiabatic switching of the interactions the exact eigenstates of the interacting system are generated from the eigenstates of the noninteracting system.

$$\hat{H} = \hat{H}_0 + e^{-\epsilon|t|}\hat{H}_1, \tag{A.1}$$

where $\epsilon > 0$. If $t = \pm\infty$ we have soluble noninteracting problem. At $t = 0$ we have a interacting system.

In the Schrödinger picture

$$|\hat{\Phi}(t)\rangle = \hat{U}_\epsilon(t, t_0)|\hat{\Phi}(t_0)\rangle \tag{A.2}$$

where the time-evolution operator is given by

$$\hat{U}_\epsilon(t, t_0) = \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 ... \int_{t_0}^{t} dt_n e^{-\epsilon(|t_1|+...+|t_n|)} \mathrm{T}[\hat{H}_1(t_1)...\hat{H}_n(t_n)] \tag{A.3}$$

In the limit $t \to \pm\infty$ the interaction picture state vector reduces to

$$|\hat{\Psi}_I(t_0)\rangle = e^{i\hat{H}_0 t_0}|\hat{\Psi}_S(t_0)\rangle = |\hat{\Phi}\rangle \tag{A.4}$$

i.e. the interaction state vector becomes time-independent. Everything develops fine and remains meaningful if $|t| < \epsilon^{-1}$ and the question is what happens when $\epsilon \to 0$. In this limit the Gell-Mann and Low theorem provides that we get meaningful results.

Gell-Man and Low theorem states that if the following quantity exists to all order in perturbation theory

$$\lim_{t\to 0} \frac{\hat{U}_\epsilon(0, -\infty)|\phi_0\rangle}{\langle\Phi_0|\hat{U}_\epsilon(0, -\infty)|\Phi_0\rangle} \tag{A.5}$$

then it is a eigenstate of $\hat{H}$

$$\hat{H}\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = E\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \tag{A.6}$$

Using this theorem we can generate the eigenstates of the interacting system adiabatically from $|\hat{\Phi}\rangle$ as the interaction is turned on.

Appendix B:
Useful commutator relations

This chapter is meant to be a short review of second quantization and the main purpose of this is to present the proofs for commutators appearing in the derivation of the equation of motion of the Green function.

Using the language of second quantization where particles can be interpreted as a excitations of the field e.g. fermions are the excitations of the fermion-field. The field operators are defined as follows

$$\hat{\psi}^\dagger(x) = \sum_n \phi^*(x)\hat{c}_n^\dagger(t) \qquad \hat{\psi}(x) = \sum_n \phi(x)\hat{c}_n(t) \tag{B.1}$$

where $\hat{c}^\dagger(t)$ and $\hat{c}(t)$ are the creation and annihilation operators in the suitable basis. These operators obey anti-commutator relations for fermions and commutator relations for bosons. Therefore the field operators obey the same relations. For example, for fermion-field operators the anti-commutator relations reads as

$$\begin{aligned} \{\hat{\psi}^\dagger(x), \hat{\psi}(x')\} &= \delta(x - x') \\ \{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x)\} &= \{\hat{\psi}(x), \hat{\psi}(x)\} = 0. \end{aligned} \tag{B.2}$$

We can express also operators in the second quantized form. For example, the one body operator in the second quantized form is

$$\hat{O} = \sum_i \hat{o}(x_i) = \int dx \hat{\psi}(x)\hat{o}(x)\hat{\psi}^\dagger(x) \tag{B.3}$$

Proof.

$$\begin{aligned} \int dx \hat{\psi}(x)\hat{o}(x)\hat{\psi}^\dagger(x)|\hat{\psi}_n\rangle &= \int dx \hat{\psi}(x)\hat{o}(x')\hat{\psi}^\dagger(x')|\hat{\psi}_n\rangle\Big|_{x=x'} \\ \int dx \hat{o}(x') \sum_{j=1}^{n} \delta(x' - x_n)\hat{\psi}_n(x_1, ..., x_{j-1}, x', x_{j+1}, ..., x_n)\Big|_{x=x'} \\ = \sum_{j=1}^{n} \hat{o}(x_j)\hat{\psi}_n(x_1, .., x_n) &= \sum_j \hat{o}(x)|\hat{\psi}_n\rangle \end{aligned}$$

□

In a similar way we can define expressions for kinetic, potential and particle density operator, which are

$$\hat{T} = -\sum_i \frac{1}{2}\nabla_i^2 = -\frac{1}{2}\int dx\hat{\psi}(x)\nabla^2\hat{\psi}^\dagger(x) \tag{B.4}$$

$$\hat{V}(t) = \sum_i v(x,t) = \int dx\hat{\psi}(X)v(x,t)\hat{\psi}^\dagger(x) \tag{B.5}$$

$$\hat{n}(x) = \sum_i \delta(x-y) = \hat{\psi}(x)\hat{\psi}^\dagger(x) \tag{B.6}$$

The Hamiltonian in the second quantized form is as follows

$$\hat{H}(t) = \int dx\hat{\psi}^\dagger(x)\hat{h}(x,t)\hat{\psi}(x) + \frac{1}{2}\int dxdy\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)w(x,y)\hat{\psi}(y)\hat{\psi}(x). \tag{B.7}$$

Using following commutator relations this can be proved. First we calculate a commutator between arbitrary one particle operator and destruction operator $\hat{\psi}(x)$.

$$\left[\hat{\psi}(x), \hat{O}\right] = \hat{O}(x)\hat{\psi}(x) \tag{B.8}$$

Proof.

$$\left[\hat{\psi}(x), \int dy\hat{\psi}^\dagger(y)\hat{o}(y)\hat{\psi}(y)\right] = \left[\hat{\psi}(x), \int dz\hat{\psi}^\dagger(y)\hat{o}(z)\hat{\psi}(z)\right] \mid_{y=z}$$

$$\int dz[\hat{\psi}(x), \hat{\psi}^\dagger(y)\hat{\psi}(x)]\hat{o}(z) \mid_{y=z}$$

$$= \int dz\hat{o}(z)\delta(x-y)\hat{\psi}(z) \mid_{z=y} = \int dy\hat{o}(y)\delta(x-y)\hat{\psi}(y) = \hat{o}(x)\hat{\psi}(x)$$

□

Next we calculate the commutator between two-particle interaction and operator $\hat{\psi}(x)$.

$$\left[\hat{\psi}(x), \hat{W}\right] = \int dzw(y,z)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y) \tag{B.9}$$

Proof.

$$\begin{aligned}
&\left[\hat{\psi}(x), \frac{1}{2}\int dydzw(y,z)\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(sy)\right] \\
&= \frac{1}{2}\int dydz\left[\hat{\psi}(x), \hat{\psi}^\dagger(y)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y)\right] w(x,z) \\
&= \frac{1}{2}\int dydz\left[\delta(x-y)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y) + \delta(x-z)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(z)\right] w(x,z) \\
&= \frac{1}{2}dzw(y,z)\left[\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y) + \hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y)\right] \\
&= \int dyw(y,z)\hat{\psi}^\dagger z\hat{\psi}(z)\hat{\psi}(y)
\end{aligned}$$

□

In the previous proof we used a following commutator relation

$$\begin{aligned}
\left[\hat{\psi(x)}, \hat{\psi}^\dagger(y)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y)\right] &= \delta(x-y)\hat{\psi}^\dagger(z)\hat{\psi}(z)\hat{\psi}(y) \\
&+\delta(x-z)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(z).
\end{aligned} \tag{B.10}$$

In a similar way the commutator relations between the creation operator $\hat{\psi}^\dagger(x)$ can also be derived. The results are

$$\left[\hat{\psi}^\dagger(x), \hat{O}\right] = -\hat{O}(x)\hat{\psi}^\dagger(x) \tag{B.11}$$

and between two-particle interaction

$$\left[\hat{\psi}^\dagger(x), \hat{W}\right] = -\int dzw(x,z)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(z)\hat{\psi}(y). \tag{B.12}$$

The equation of motion for the field operator $\hat{\psi}(x)$ is then

$$i\partial_t\hat{\psi}(x) = \left[\hat{\psi}(x), \hat{H}(t)\right] = \hat{h}(x)\hat{\psi}(x) + \int dyw(x,y)\hat{\psi}^\dagger\hat{\psi}(y)\hat{\psi}(x). \tag{B.13}$$

Appendix C: Properties of time-evolution operator

C.1 Properties of $\hat{U}$

Unitary property reads as

$$\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0). \tag{C.1}$$

From the unitary property it follows that

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = 1, \tag{C.2}$$

which in some cases is taken to be the definition of the unitary property.

Time-evolution at equal time arguments is equal to one

$$\begin{gathered} |\hat{\Psi}(t)\rangle = \hat{U}(t,t)|\hat{\Psi}(t)\rangle = |\hat{\Psi}(t)\rangle \\ \Rightarrow \hat{U}(t,t) = 1. \end{gathered} \tag{C.3}$$

Because the time-evolution operators form a group, a multiplication of two group members gives a new member of the group i.e.

$$\hat{U}(t_1,t_2)\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3). \tag{C.4}$$

The adjoint of $\hat{U}$

$$\hat{U}(t,t_0)\hat{U}(t_0,t) = 1 \Rightarrow \hat{U}(t_0,t) = \hat{U}^\dagger(t,t_0) \tag{C.5}$$

C.2 Proof of equation (2.6)

Differentiate first the equation $|\hat{\Psi}(t)\rangle = \hat{U}(t,t')|\hat{\Psi}(t')\rangle$ with respect to t. This gives following

$$\begin{gathered} \partial_t|\hat{\Psi}(t)\rangle = -i\hat{H}(t)|\hat{\Psi}(t)\rangle = i\hat{H}(t)\hat{U}(t,t')|\hat{\Psi}(t')\rangle = \partial_t\hat{U}(t,t')|\hat{\Psi}(t')\rangle \\ \Rightarrow \partial_t\hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t') \end{gathered} \tag{C.6}$$

because the state $|\hat{\Psi}(t)\rangle$ was arbitrary. Differentiation with respect to t' gives

$$\partial_{t'}\hat{U}(t,t') = -\hat{U}(t,t')\hat{H}(t') \tag{C.7}$$

As a conclusion the time-evolution operator satisfies the following set of equations with the boundary condition.

$$i\partial_t\hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t') \tag{C.8}$$
$$i\partial_{t'}\hat{U}(t,t') = -\hat{U}(t,t')\hat{H}(t') \tag{C.9}$$
$$\hat{U}(t,t) = 1 \tag{C.10}$$

Integrating equation (C.8) from t to t' gives $(t > t')$

$$\begin{aligned} i\int_{t'}^{t} d\tilde{t}\hat{U}(\tilde{t},t) = \hat{U}(t,t') - 1 = \int_{t'}^{t} d\tilde{t}\hat{H}(\tilde{t})\hat{U}(\tilde{t},t') \\ \Rightarrow \hat{U}(t,t') = 1 - i\int_{t'}^{t} d\tilde{t}\hat{H}(\tilde{t})\hat{U}(\tilde{t},t'). \end{aligned} \tag{C.11}$$

This equation can be iterated further to get an infinite series

$$\begin{aligned} \hat{U}(t,t') = 1 - i\int_{t'}^{t} d\tilde{t}_1\hat{H}(\tilde{t}_1)\hat{U}(\tilde{t}_1,t') + (-i)^2\int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2) \\ +(-i)^3\int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\int_{t'}^{\tilde{t}_2} d\tilde{t}_3\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2)\hat{H}(\tilde{t}_3) + ... \end{aligned} \tag{C.12}$$

Next look for example the second order term, it can be rewritten as follows

$$\begin{aligned} \int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2)\hat{U}(\tilde{t}_2,t') = \\ \int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2) + \int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2). \end{aligned} \tag{C.13}$$

Changing the name of dummy integration variables gives the second term as follows

$$\int_{t'}^{t} d\tilde{t}_1\int_{t}^{t'} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2) = \int_{t'}^{t} d\tilde{t}_2\int_{t'}^{\tilde{t}_2} d\tilde{t}_1\hat{H}(\tilde{t}_2)\hat{H}(\tilde{t}_1). \tag{C.14}$$

This gives for the result

$$\begin{aligned} \int_{t'}^{t} d\tilde{t}_1\int_{t'}^{\tilde{t}_1} d\tilde{t}_2\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2)\hat{U}(\tilde{t}_2,t') \\ = \int_{t'}^{t} d\tilde{t}_1\int_{t'}^{t} d\tilde{t}_2\left[\theta(t_1,t_2)\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2) + \theta(t_2,t_1)\hat{H}(\tilde{t}_2)\hat{H}(\tilde{t}_1)\right]. \end{aligned} \tag{C.15}$$

Writing this by using the time-ordering operator $\mathcal{T}_\mathcal{C}$ on the contour

$$\int_{t'}^{t} d\tilde{t}_1 \int_{t'}^{\tilde{t}_1} d\tilde{t}_2 \hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2) = \int_{t'}^{t} d\tilde{t}_1 \int_{t'}^{t} d\tilde{t}_2 \mathcal{T}_\mathcal{C}[\hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2)]. \tag{C.16}$$

Straightforward generalization gives the final result

$$\hat{U}(t,t') = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} d\tilde{t}_1 \int_{t'}^{t} d\tilde{t}_2 ... \int_{t'}^{t} d\tilde{t}_n \mathcal{T}_\mathcal{C}[\hat{H}(\tilde{t}_1)...\hat{H}(\tilde{t}_n])]. \tag{C.17}$$

Appendix D: Kubo-Martin-Schwinger boundary conditions

We define the Green functions as an ensemble average of the time-ordered product of of annihilation and creation operators as

$$\mathbf{G}_{mn}(z,z') \equiv i\Big\langle \mathcal{T}\big[c_m(z)\bar{c}_n(z')\big]\Big\rangle. \tag{D.1}$$

The time-ordering is done on the Keldysh contorur γ (see Fig. 2.1). The variable $z = t + \tau \in \mathtt{C}$ is running on γ, $t = \mathrm{Re}[z]$ and $\tau = \mathrm{Im}[z]$ and A, B are endpoints of the contour γ. $c_m(z)$ and $\bar{c}_n(z)$ are Heisenberg operators defined by nonunitary evolution operator for complex times z. On the vertical track $\hat{H}_u(t) = 0$ ($\hat{H}_U(t) = \sum_{mn} U_{mn}\bar{c}_m c_n = 0$ if $t \leq 0$) $\Rightarrow \hat{K}(\tau) = \hat{T} + \hat{U}(\tau) = \hat{T} = \hat{K}(0)$ independent of τ.

The Green function satisfies the Kubo-Martin-Schwinger boundary conditions

$$\begin{aligned}
\mathbf{G}(A,z') &= i\Big\langle \mathcal{T}\big[c_m(A)\bar{c}_n(z')\big]\Big\rangle = i\frac{\mathrm{Tr}\left\{e^{-\beta(\hat{K}-\mu\hat{N})}\mathcal{T}\big[c_m(A)\bar{c}_n(z')\big]\right\}}{\mathrm{Tr}\left\{e^{-\beta(\hat{K}-\mu\hat{N})}\right\}} \\
&= i\frac{\mathrm{Tr}\left\{c(A)e^{-\beta(\hat{K}-\mu\hat{N})}\bar{c}(z')\right\}}{Z_G} = i\frac{\mathrm{Tr}\left\{e^{-\beta\hat{K}}c(B)e^{\hat{K}\beta}e^{-\beta\hat{K}}e^{\beta\mu\hat{N}}\bar{c}(z')\right\}}{Z_G} \\
&= i\frac{\mathrm{Tr}\left\{e^{-\hat{K}\beta}e^{\mu(N+1)\beta}c(B)\bar{c}(z')\right\}}{Z_G} \\
&= -e^{\beta\mu}\mathbf{G}(B,z')
\end{aligned} \tag{D.2}$$

and

$$\begin{aligned}
\mathbf{G}(z,A) &= i\Big\langle \mathcal{T}\big[c_m(z)\bar{c}_n(A)\big]\Big\rangle = i\frac{\mathrm{Tr}\left\{e^{-\beta(\hat{K}-\mu\hat{N})}\mathcal{T}\big[c_m(z)\bar{c}_n(A)\big]\right\}}{\mathrm{Tr}\left\{e^{-\beta(\hat{K}-\mu\hat{N})}\right\}} \\
&= i\frac{\mathrm{Tr}\left\{\bar{c}(A)e^{-\beta(\hat{K}-\mu\hat{N})}c(z)\right\}}{Z_G} = i\frac{\mathrm{Tr}\left\{e^{-\beta\hat{K}}c(B)e^{\hat{K}\beta}e^{-\beta\hat{K}}e^{\beta\mu\hat{N}}\bar{c}(z)\right\}}{Z_G} \\
&= i\frac{\mathrm{Tr}\left\{e^{-\beta\hat{K}}e^{\beta\mu(N-1)}\bar{c}(B)c(z)\right\}}{Z_G} \qquad \text{(D.3)} \\
&= -e^{-\beta\mu}\mathbf{G}(z,B), \qquad \text{(D.4)}
\end{aligned}$$

where we used following information $\left(Z_G = \mathrm{Tr}\left\{e^{-\beta(\hat{K}-\mu\hat{N})}\right\}\right)$, $\hat{c}f(N) = f(N+1)\hat{c}$ and $\hat{c}^\dagger f(N) = f(N-1)\hat{c}^\dagger$.

Appendix E:
Proofs for equations appearing in the derivation of 2B approximation

E.1 Proof of equation (4.62)

Action is defined as

$$S = i\ln\left[\hat{U}(t_0 - i\beta, t_0)\right] \tag{E.1}$$

where

$$U(t,t') = \mathrm{T}_C\left[\exp\left(-i\int_{t'}^{t} d\tilde{t}\hat{H}(\tilde{t})\right)\right] \tag{E.2}$$

The equation of motion for time-evolution operator were

$$\partial_t \hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t') \tag{E.3}$$

$$\partial_{t'} \hat{U}(t,t') = -\hat{U}(t,t')\hat{H}(t') \tag{E.4}$$

$$\hat{U}(t,t) = 1 \tag{E.5}$$

Small perturbation $\delta\hat{V}(t)$

$$i\partial_t \delta\hat{U}(t,t') = \delta\hat{H}(t)\hat{U}(t,t') + \hat{H}(t)\delta\hat{U}(t,t') \tag{E.6}$$

$$i\partial_{t'} \delta\hat{U}(t,t') = -\delta\hat{U}(t,t')\hat{H}(t') - \hat{U}(t,t')\delta\hat{H}(t') \tag{E.7}$$

$$\delta\hat{U}(t,t) = 0 \tag{E.8}$$

multiply with $\hat{U}(t',t)$

$$\begin{aligned} i\hat{U}(t,t')\partial\hat{U}(t,t') &= \hat{U}(t',t)\delta\hat{V}(t)U(t,t') + \hat{U}(t',t)\hat{H}(t)\delta\hat{U}(t,t') \\ &= \hat{U}(t',t)\delta\hat{V}(t)U(t,t') - i\partial_t\hat{U}(t',t)\hat{U}(t,t') \end{aligned} \tag{E.9}$$

$$i\partial_t[\hat{U}(t',t)\delta\hat{U}(t,t')] = \hat{U}(t',t)\delta\hat{V}(t)\hat{U}(t,t') \tag{E.10}$$

$$\delta\hat{U}(t,t') = \int_{t'}^{t} d\tau\hat{U}(t,\tau)\delta\hat{V}(\tau)\hat{U}(\tau,t') \tag{E.11}$$

E.2 Proof of equation (4.64)

We will need to calculate functional derivatives respect to perturbation v, therefore we firs work it out.

$$\frac{\delta\hat{U}(t_0-i\beta,t_0)}{\delta v(xt)}=\frac{\delta}{\delta v(xt)}\int_{t_0}^{t_0-i\beta}d\tau\hat{U}(t_0-i\beta,t)\delta\hat{V}(t)\hat{U}(\tau,t_0) \tag{E.12}$$

Assuming that the perturbation has a form

$$\delta\hat{V}(t)=\int dy\delta v(yt)\hat{n}(y) \tag{E.13}$$

we get

$$\frac{\delta\hat{U}(t_0-i\beta,t_0)}{\delta v(xt)}=\frac{\delta}{\delta v(xt)}\int_{t_0}^{t_0-i\beta}d\tau\int dy\hat{U}(t_0-i\beta,t)\hat{n}(y)\delta(x-y)\delta(\tau,t)\delta\hat{U}(\tau,t_0) \tag{E.14}$$

so that we have

$$\frac{\delta\hat{U}(t_0-i\beta,t_0)}{\delta v(xt)}=\hat{U}(t_0-i\beta,t)n(x)\hat{U}(\tau,t_0)=\hat{U}(t-i\beta,t)\hat{n}_H(xt). \tag{E.15}$$

Next we prove that the change of the expectation value of the time-ordered product of two operators is

$$\frac{\delta\langle\mathrm{T}_C[\hat{A}(1)\hat{B}(2)]\rangle}{\delta v(3)}=-i\langle\mathrm{T}_C[\hat{A}(1)\hat{B}(2)\hat{n}(3)]\rangle+i\langle\mathrm{T}_C[\hat{A}(1)\hat{B}(2)]\rangle\langle\hat{n}(3)\rangle \tag{E.16}$$

Nevertheless the change of expectation value of an arbitrary operator $\hat{O}(t)$ is proven just because it simpler to type. The previous result follows from the following derivation straightforwardly.

$$\begin{aligned}\frac{\delta\langle\hat{O}(t)\rangle}{\delta v(3)}=&-\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_2)\hat{n}(2)\hat{U}(t_2,t_1)\hat{O}(t_1)\hat{U}(t_1,t_0)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\theta(t_2,t_1)\\&-\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_1)\hat{O}(t_1)\hat{U}(t_1,t_2)\hat{n}(2)\hat{U}(t_2,t_0)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\theta(t_1,t_2)\\&+\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_1)\hat{O}(t_1)\hat{U}(t_1,t_0)\right\}}{\left[\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}\right]^2}\cdot\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_2)\hat{n}(2)\hat{U}(t_2,t_0)\right\}\end{aligned} \tag{E.17}$$

Writing operators back to Heisenberg representation gives

$$\begin{aligned}\frac{\delta\langle\hat{O}(t)\rangle}{\delta v(3)} = &-\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\hat{n}_H(2)\hat{O}_H(t_1)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\theta(t_2,t_1)\\ &-\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\hat{O}_H(t_1)\hat{n}_H(2)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\theta(t_1,t_2)\\ &+\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\hat{O}_H(t_1)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\frac{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\hat{n}_H(2)\right\}}{\mathrm{Tr}\left\{\hat{U}(t_0-i\beta,t_0)\right\}}\end{aligned} \tag{E.18}$$

or shortly written

$$\begin{aligned}\frac{\delta\langle\hat{O}(t)\rangle}{\delta v(3)} = &-i\theta(t_1,t_2)\langle\hat{O}_H(t_1)\hat{n}_H(2)\rangle - i\theta(t_2,t_1)\langle\hat{n}_H(2)\hat{O}(t_1)\rangle\\ &+i\langle\hat{O}_H(t_1)\rangle\langle\hat{n}_H(2)\rangle\end{aligned} \tag{E.19}$$

Next we define fluctuation/deviation operator which measures the deviations away from the average

$$\Delta\hat{O}_H(xt) = \hat{O}_H(xt) - \langle\hat{O}_H(xt)\rangle \tag{E.20}$$

Using this definiton we have

$$\begin{aligned}\frac{\delta\langle\hat{O}(t)\rangle}{\delta v(3)} = &-i\theta(t_1,t_2)\langle\Delta\hat{O}_H(t_1)\Delta\hat{n}_H(2)\rangle - i\theta(t_1,t_2)\langle\Delta\hat{O}_H(t_1)\rangle\langle\hat{n}_H(2)\rangle\\ &-i\theta(t_1,t_2)\langle\hat{O}_H(t_1)\rangle\langle\Delta\hat{n}_H(2)\rangle - i\theta(t_1,t_2)\langle\hat{O}_H(t_1)\rangle\langle\hat{n}_H(2)\rangle\\ &-i\theta(t_2,t_1)\langle\Delta\hat{O}_H(t_1)\Delta\hat{n}_H(2)\rangle - i\theta(t_2,t_1)\langle\hat{n}_H(2)\rangle\langle\Delta\hat{O}_H(t_1)\rangle\\ &-i\theta(t_2,t_1)\langle\Delta\hat{n}_H(2)\rangle\langle\hat{O}_H(t_1)\rangle - i\theta(t_2,t_1)\langle\hat{n}_H(2)\rangle\langle\hat{O}_H(t_1)\rangle\end{aligned} \tag{E.21}$$

Simplifying we finally get

$$\frac{\delta\langle\hat{O}(t)\rangle}{\delta v(3)} = -i\left\langle \mathrm{T}_C\left[\Delta\hat{O}_H(t_1)\Delta\hat{n}_H(2)\right]\right\rangle \tag{E.22}$$

Appendix F:
Proofs for equations appearing in the derivation of GW approximation

F.1 Form of screened interaction, polarization propagator and self-energy

Starting from the equation definition of the screened Coulomb interaction and using the definition of V we have

$$\begin{aligned} W(1,2) &= \int d3w(1,3)\frac{\delta V(2)}{\delta v(3)} \\ &= \int d3w(1,3)\frac{\delta}{\delta v(3)}\left[v(2) - i\int d4w(2,4)G(4,4^+)\right] \end{aligned} \tag{F.1}$$

Simplifying a little

$$\begin{aligned} W(1,2) &= \int d3w(1,3)\delta(2,3) - i\int d3d4w(2,4)\frac{\delta G(4,4+)}{\delta v(3)}w(1,3) \\ &= w(1,3) + i\int d3d4d5d6w(1,3)w(2,4)G(4,5)\frac{\delta G^{-1}(5,6)}{\delta v(3)}G(6,4^+). \end{aligned} \tag{F.2}$$

With the help of the following identity

$$\frac{\delta}{\delta v(1)} = \int \frac{\delta V(2)}{\delta v(1)}\frac{\delta}{\delta V(2)}d2 \tag{F.3}$$

we get

$$\begin{aligned} W(1,2) &= w(1,2) + i\int d3d4d5w(1,3)w(2,4)G(4,5)\int d7\frac{\delta V(7)}{\delta v(3)}\frac{\delta G^{-1}(5,6)}{\delta V(7)}G(6,4^+) \\ &= w(1,2) + i\int d3d4d5d7w(2,4)W(1,7)G(4,5)\frac{\delta G^{-1}(5,6)}{\delta w(7)}G(6,4^+). \end{aligned} \tag{F.4}$$

Thus the screened interaction has the form

$$W(1,2) = w(1,2) + i \int d3d4d5d7 w(2,4) W(1,7) P(4,7) \tag{F.5}$$

where we have defined the polarization propagator as

$$P(4,7) = \int d5d6 G(4,5) \frac{\delta G^{-1}(5,6)}{\delta w(7)} G(6,4^+). \tag{F.6}$$

Writing self-energy in terms of vertex-function and screened interaction is quite straightforward

$$\begin{aligned} \Sigma(1,2) &= -i \int d3d4 w(1,3) G(1,4) \frac{\delta G^{-1}(4,2)}{\delta v(3)} \\ &= -i \int d3d4 w(1,3) \frac{\delta G^{-1}(4,2)}{\delta V(3^+)} \frac{\delta V(3^+)}{\delta v(3)} \end{aligned} \tag{F.7}$$

with use of definitions of Γ and W

$$\Gamma(12;3) = -\frac{\delta G^{-1}(1,2)}{\delta v(3)} \tag{F.8}$$

$$W(1,2) = \int d3 w(1,3) \frac{\delta V(2)}{\delta v(3)} \tag{F.9}$$

we get

$$\Sigma(1,2) = i \int d3d4 W(1,3^+) G(1,4) \Gamma(42;3) \tag{F.10}$$

F.2 Functional derivatives of G and W respect to potential V

Let us first calculate what is $\delta G / \delta V$

$$\frac{\delta G(1,2)}{\delta V(3)} = -\frac{\delta G(1,2)}{\delta v(3)} \frac{\delta v(3)}{\delta V(3)} = \int d4d5 G(1,4) \frac{\delta G^{-1}(4,5)}{\delta v(3)} G(5,2) \frac{\delta v(3)}{\delta V(3)} \tag{F.11}$$

from this it follows that

$$\begin{aligned} \frac{\delta G(1,2)}{\delta V(3)} &= \int d4d5 G(1,4) \frac{\delta G^{-1}(4,5)}{G}(1,5) \\ &= \int d4d5 G(1,4) \Gamma(4,5;3) \delta v(3) G(1,5). \end{aligned} \tag{F.12}$$

Next we calculate what is $\delta W/\delta V$.

$$W(1,2) = w(1,2) + i \int d3d4d5d7w(2,4)W(1,7)P(4,7) \tag{F.13}$$

Writing the equation of W formally as

$$W(1,2) = w(1,2) + W(1,3)P(3,4)w(4,2) \Rightarrow W = w + WPw \tag{F.14}$$

Let us write this a little bit differently

$$W(1-Pw) = w \Rightarrow W = w(1-Pw)^{-1} \Rightarrow W[w(1-Pw)^{-1}]^{-1} = WW^{-1} = 1. \tag{F.15}$$

Differentiating WW^{-1} respect to V

$$\begin{aligned} \frac{\delta(WW^{-1})}{\delta V} &= \frac{\delta W}{\delta V}W^{-1} + W\frac{\delta W^{-1}}{\delta V} = 0 \\ \Rightarrow \frac{\delta W}{\delta V} &= -W\frac{\delta W}{\delta V}W. \end{aligned} \tag{F.16}$$

From this it follows with definition $W^{-1} = w^-1(1-Pw)$ that

$$\frac{\delta W}{\delta V} = -W\frac{\delta w^{-1}(1-Pw)}{\delta V}W = W\frac{\delta P}{\delta V}W \tag{F.17}$$

The derivative of W respect to V is therefore

$$\frac{\delta W(1,2)}{\delta V(3)} = \int d3d5W(1,4)\frac{\delta P(4,)}{\delta V(3)}W(5,2). \tag{F.18}$$

Appendix G:
G Proofs for equations appearing in derivation of steady-state current

G.1 Langreth Rules

By using the Langreth rules [20] we can extract the greater and lesser components of the Green function. Let's do the lesser component as an example.

$$\begin{aligned}
\mathbf{G}^<(z,z') &= \mathbf{g}^<(z,z') + \int_0^z \mathrm{d}\bar{z}\mathbf{g}^>(z,\bar{z})\mathbf{V}(\bar{z})\mathbf{G}^<(\bar{z},z') + \int_z^{z'} \mathrm{d}\bar{z}\mathbf{g}^<(z,\bar{z})\mathbf{V}(\bar{z})\mathbf{G}^<(\bar{z},z') \\
&+ \int_{z'}^0 \mathrm{d}\bar{z}\mathbf{g}^<(z,\bar{z})\mathbf{V}(\bar{z})\mathbf{G}^>(\bar{z},z') + \int_0^{-i\beta} \mathrm{d}\bar{\tau}\mathbf{g}^<(z,-i\bar{\tau})\mathbf{V}(-i\bar{\tau})\mathbf{G}^>(-i\bar{\tau},z') \\
\Rightarrow \mathbf{G}^<(t,t') &= \mathbf{g}^<(t,t') + \int_0^t \mathrm{d}\bar{t}\mathbf{g}^>(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t') + \int_t^{t'} \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t') \\
&+ \int_{t'}^0 \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^>(\bar{t},t') + \int_0^{-i\beta} \mathrm{d}\bar{\tau}\mathbf{g}^<(t,-i\bar{\tau})\mathbf{V}(-i\bar{\tau})\mathbf{G}^>(-i\bar{\tau},t').
\end{aligned} \tag{G.1}$$

Performing a change of variables $\mathrm{d}\bar{\tau} = -i\mathrm{d}\tau$ we get

$$\begin{aligned}
\mathbf{G}^<(t,t') &= \mathbf{g}^<(t,t') + \int_0^t \mathrm{d}\bar{t}\mathbf{g}^>(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t') + \int_t^{t'} \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t') \\
&\quad + \int_{t'}^0 \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^>(\bar{t},t') + \int_0^{\beta} \mathrm{d}\bar{\tau}\mathbf{g}^<(t,\tau)\mathbf{V}(\tau)\mathbf{G}^>(\tau,t') \qquad \text{(G.2)} \\
&= \mathbf{g}^<(t,t') + \int_0^t \mathrm{d}\bar{t}[\mathbf{g}^>(t,\bar{t}) - \mathbf{g}^<(t,\bar{t})]\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t) \\
&\quad - \int_0^{t'} \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\mathbf{V}(\bar{t})[\mathbf{G}^<(\bar{t},t') - \mathbf{G}^>(\bar{t},t')] + i\int_0^{\beta} \mathrm{d}\tau\mathbf{g}^\rceil(t,\tau)\mathbf{V}(\tau)\mathbf{G}^\lceil(\tau,t')
\end{aligned} \tag{G.3}$$

On a next step we need to use the relations between retarded / advanced Green function and the greater / lesser Green functions

$$\mathbf{G}^R = \theta(t-t')\left[\mathbf{G}^>(t,t') - \mathbf{G}^<(t,t')\right] \tag{G.4}$$
$$\mathbf{G}^A = \theta(t'-t)\left[\mathbf{G}^<(t,t') - \mathbf{G}^>(t,t')\right]. \tag{G.5}$$

$$\begin{aligned}\mathbf{G}^<(t,t') &= \int_0^\infty \mathrm{d}\bar{t}[\mathbf{g}^>(t,\bar{t}) - \mathbf{g}^<(t,\bar{t})]\mathbf{V}(\bar{t})\mathbf{G}^<(\bar{t},t) + i\int_0^\beta \mathrm{d}\tau \mathbf{g}^\rceil(t,\tau)\mathbf{V}(\tau)\mathbf{G}^\lceil(\tau,t') \\ &+ \int_0^\infty \mathrm{d}\bar{t}\theta(\bar{t},t)\mathbf{g}^<(t,\bar{t})\left[\delta(\bar{t},t')\theta(t,\bar{t})\mathbf{V}(\bar{t})[\mathbf{G}^<(\bar{t},t') - \mathbf{G}^>(\bar{t},t')]\right] \qquad \text{(G.6)} \\ &= \int_0^\infty \mathrm{d}\bar{t}\mathbf{g}^<(t,\bar{t})\left[\delta(\bar{t},t') + \mathbf{V}(\bar{t})\mathbf{G}^A(\bar{t},t')\right] + \int_0^\infty \mathrm{d}\bar{t} + \mathbf{g}^R(t,\bar{t}\mathbf{V}(\bar{t}))\mathbf{G}^<(\bar{t},t') \\ &+ i\int_0^\beta \mathrm{d}\tau \mathbf{g}^\rceil(t,\tau)\mathbf{V}(\tau)\mathbf{G}^\lceil(\tau,t'). \qquad \text{(G.7)}\end{aligned}$$

By introducing the following short hand notation

$$\star = i\int_0^\beta \mathrm{d}\tau \qquad\qquad \cdot = \int_0^\infty \mathrm{d}t \tag{G.8}$$

the result can be written as

$$\mathbf{G}^< = \mathbf{g}^< \cdot (\delta + \mathbf{V}\cdot\mathbf{G}^A) + \mathbf{g}^R\cdot\mathbf{V}\cdot G^< + \mathbf{g}^\rceil \star \mathbf{V}\star\mathbf{G}^\lceil. \tag{G.9}$$

The greater component can be obtained in a similar way and the result is

$$\mathbf{G}^> = \mathbf{g}^> \cdot (\delta + \mathbf{V}\cdot\mathbf{G}^A) + \mathbf{g}^R\cdot\mathbf{V}\cdot\mathbf{G}^> + \mathbf{g}^\rceil \star \mathbf{V}\star\mathbf{G}^\lceil. \tag{G.10}$$

Retarded and advanced components:

$$\mathbf{G}^{R,A} = \pm\theta(\pm t \mp t')\left[\mathbf{G}^>(t,t') - \mathbf{G}^<(t,t')\right] \tag{G.11}$$

Combining the equations (G.9) and (G.10) and assuming that $t > t'$ we get

$$\begin{aligned}
\mathbf{G}^{>}(t,t') - \mathbf{G}^{<}(t,t') &= \mathbf{g}^{>}(t,t') - \mathbf{g}^{<}(t,t') + \int_0^t \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\big[\mathbf{G}^{>}(\bar{t},t') - \mathbf{G}^{<}(\bar{t},t')\big] \\
&\quad + \int_0^{t'} \mathrm{d}\bar{t}\big[\mathbf{g}^{>}(t,\bar{t}) - \mathbf{g}^{<}(t,\bar{t})\big]\mathbf{V}(t)\mathbf{G}^A(\bar{t},t') \qquad \text{(G.12)} \\
&= \mathbf{g}^{>}(t,t') - \mathbf{g}^{<}(t,t') + \int_0^{t'} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\big[\mathbf{G}^{>}(\bar{t},t') - \mathbf{G}^{<}(\bar{t},t')\big] \\
&\quad + \int_{t'}^{t} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\big[\mathbf{G}^{>}(\bar{t},t') - \mathbf{G}^{<}(\bar{t},t')\big] \\
&+ \int_0^{t'} \mathrm{d}\bar{t}\big[\mathbf{g}^{>}(t,\bar{t}) - \mathbf{g}^{<}(t,\bar{t})\big]\mathbf{V}(t)\mathbf{G}^A(\bar{t},t') \qquad \text{(G.13)} \\
&= \mathbf{g}^{>}(t,t') - \mathbf{g}^{<}(t,t') + \int \mathrm{d}\bar{t} + \int_0^{t'} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\theta(\bar{t}-t')\mathbf{G}^R(\bar{t},t') \\
&\quad - \int_0^{t'} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^A(\bar{t},t')\theta(-t+t') \\
&\quad + \int_0^{t'} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^A(\bar{t},t')\theta(-t+t') \\
&= \mathbf{g}^R(t,t') + \int_0^{\infty} \mathrm{d}\bar{t}\mathbf{g}^R(t,\bar{t})\mathbf{V}(\bar{t})\mathbf{G}^R(\bar{t},t') \qquad \text{(G.14)} \\
&= \mathbf{g}^R \cdot (\delta + \mathbf{V}\cdot\mathbf{G}^R) \qquad \text{(G.15)}
\end{aligned}$$

In a similar fashion we can derive the expression for $-\mathbf{G}^{>}(t,t') + \mathbf{G}^{<}(t,t')$ which together with Eq. (G.15) lead to

$$\mathbf{G}^{R,A} = \mathbf{g}^{R,A} + \mathbf{g}^{R,A}\cdot\mathbf{V}\cdot\mathbf{G}^{R,A} \qquad \text{(G.16)}$$

The equations (G.9) and (G.10) can be solved for the $\mathbf{G}^{\gtrless}(t,t')$ respectively. For example for the $\mathbf{G}^{>}(t,t')$ we start by multiplying the equation (G.10) from the left with $\delta - \mathbf{g}^R\cdot\mathbf{V}$

$$\begin{aligned}
\Rightarrow (\delta - \mathbf{g}^R\cdot\mathbf{V})\mathbf{G}^{>} &= (\delta - \mathbf{g}^R\cdot\mathbf{V})\mathbf{g}^{>}\cdot(\delta + \mathbf{V}\cdot\mathbf{G}^A) \\
&\quad + \mathbf{g}^R\cdot V\cdot\mathbf{G}^{>} + (\delta - \mathbf{g}^R\cdot\mathbf{V})\mathbf{g}^{\rceil}\star\mathbf{V}\star\mathbf{G}^{\lceil} \qquad \text{(G.17)}
\end{aligned}$$

The expression $\delta - \mathbf{g}^R\cdot\mathbf{V}$ can be shown to be equivalent with $\mathbf{g}^R\cdot(\mathbf{G}^R)^{-1}$ as follows

$$\begin{aligned}
& \mathbf{G}^{R,A} = \mathbf{g}^{R,A} + \mathbf{G}^{R,A}\cdot\mathbf{V}\cdot\mathbf{G}^{R,A} \\
\Rightarrow\ & \mathbf{G}^R = \mathbf{g}^R + \mathbf{G}^R\cdot\mathbf{V}\cdot\mathbf{G}^R \\
\Rightarrow\ & \mathbf{G}^R - \mathbf{g}^R\cdot\mathbf{V}\cdot\mathbf{G}^R = \mathbf{g}^R \\
\Rightarrow\ & (\delta - \mathbf{g}^R\cdot\mathbf{V})\cdot\mathbf{G}^R = \mathbf{g}^R\Big| \cdot (\mathbf{G}^R)^{-1} \\
\Rightarrow\ & (\delta - \mathbf{g}^R\cdot\mathbf{V}) = \mathbf{g}^R\cdot(\mathbf{G}^R)^{-1}. \qquad \text{(G.18)}
\end{aligned}$$

Now we just need to simplify a bit and we arrive to the final formula

$$\begin{aligned}
\Rightarrow \mathbf{g}^R \cdot (\mathbf{G}^R)^{-1} \cdot \mathbf{G}^> &= \mathbf{g}^< \cdot (\delta + \mathbf{V} \cdot \mathbf{G}^A) + \mathbf{g}^\rceil \star \mathbf{V} \star \mathbf{G}^\lceil \Big| \cdot \mathbf{G}^R \cdot (\mathbf{g}^R)^{-1} \\
&= (\delta + \mathbf{V} \cdot \mathbf{G}^R) \qquad \text{(G.19)} \\
\Rightarrow \mathbf{G}^R \cdot (\mathbf{g}^R)^{-1} \cdot \mathbf{g}^R \cdot (\mathbf{G}^R)^{-1} \cdot \mathbf{G}^> &= \mathbf{G}^R \cdot (\mathbf{g}^R)^{-1} \cdot \mathbf{g}^< \cdot (\delta + \mathbf{V} \cdot \mathbf{G}^A) \\
&\quad + \mathbf{G}^R \cdot (\mathbf{g}^R)^{-1} \cdot \mathbf{g}^\rceil \star \mathbf{V} \star \mathbf{G}^\lceil \qquad \text{(G.20)} \\
\Rightarrow \mathbf{G}^> &= (\delta + \mathbf{V} \cdot \mathbf{G}^A) \cdot \mathbf{g}^< \cdot (\delta + \mathbf{V} \cdot \mathbf{G}^A) \\
&\quad + (\delta + \mathbf{V} \cdot \mathbf{G}^A) \cdot \mathbf{g}^\rceil \star \mathbf{V} \star \mathbf{G}^\lceil \qquad \text{(G.21)}
\end{aligned}$$

A similar derivation applies also for $\mathbf{G}^<$ and the final result can be compactly written as

$$\therefore \mathbf{G}^\gtrless = (\delta + \mathbf{V} \cdot \mathbf{G}^A) \cdot \mathbf{g}^\gtrless \cdot (\delta + \mathbf{V} \cdot \mathbf{G}^A) + (\delta + \mathbf{V} \cdot \mathbf{G}^A) \cdot \mathbf{g}^\rceil \star \mathbf{V} \star \mathbf{G}^\lceil. \qquad \text{(G.22)}$$

We can analyze this equation a bit further. The uncontacted Green function at (t, t') can be expressed with the help or retarded and advanced components as

$$\mathbf{g}^\gtrless(t, t') = \mathbf{g}^R(t, 0)\mathbf{g}^\gtrless(0, 0)\mathbf{g}^A(0, t'). \qquad \text{(G.23)}$$

The mixed-components of the uncontacted Green function are defined as follows

$$\mathbf{g}(\tau, t) = -i\langle c(\tau)\bar{c}(t)\rangle = -i\langle c(\tau)\bar{c}\mathbf{S}^\dagger(t)\rangle = -i\mathbf{g}^\lceil(\tau, 0)\mathbf{g}^A(0.t), \qquad \text{(G.24)}$$

$$\mathbf{g}(t, \tau) = i\langle\bar{c}(\tau)c(t)\langle = i\mathbf{S}^\dagger\rangle\mathbf{c}(\tau)c(0)\rangle = i\mathbf{g}^R(t, 0)\mathbf{g}^\rceil(0, \tau). \qquad \text{(G.25)}$$

After some manipulations we get

$$\begin{aligned}
\mathbf{G}^\gtrless(t, t') &= (\delta + \mathbf{V} \cdot \mathbf{G}^R) \cdot \mathbf{g}^R(t, 0) \cdot \mathbf{g}^\gtrless \cdot \mathbf{g}^A(0, t')(\delta + \mathbf{V} \cdot \mathbf{G}^A) \\
&\quad + i(\delta + \mathbf{V} \cdot \mathbf{G}^R)\mathbf{g}^R(t, 0) \cdot \mathbf{g}^\lceil(0, \tau) \star \mathbf{V} \star \mathbf{G}^\rceil \\
&= \mathbf{G}^R(t, 0)\mathbf{g}^\gtrless(0, 0)\mathbf{G}^A(0, t') + i\mathbf{G}^R(t, 0)\mathbf{g}^\rceil(0, \tau) \star \mathbf{V} \star \mathbf{G}^\lceil \\
&= \mathbf{G}^R(t, 0)\mathbf{g}^\gtrless(0, 0)\mathbf{G}^A(0, t') + i\mathbf{G}^R(t, 0)[\mathbf{g}^\rceil + \mathbf{V} \star \mathbf{G}^\lceil](0, t) \\
&= \mathbf{G}^R(t, 0)\Big[\mathbf{g}^\gtrless(0, 0)\mathbf{G}^A(0, t') + i[\mathbf{g}^\rceil + \mathbf{V} \star \mathbf{G}^\lceil](0, t)\Big] \\
&= \mathbf{G}^R(t, 0)\Big[\mathbf{g}^\gtrless(0, 0) + i[\mathbf{g}^\rceil + \mathbf{V} \star \mathbf{G}^\lceil](\tau, t)\Big]\mathbf{G}^A(0, t') \\
&= \mathbf{G}^R(t, 0)\mathbf{G}^\gtrless(0, 0)\mathbf{G}^A(0, t'), \qquad \text{(G.26)}
\end{aligned}$$

G.2 Proof for equations (5.104) and (5.106)

The Hamiltonian was

$$H = \sum_l \varepsilon_l \hat{c}_l^\dagger \hat{c}_l + \sum_{k\alpha} \varepsilon_{k\alpha} \hat{c}_{k\alpha}^\dagger \hat{c}_{k\alpha} + \sum_{ij,mn} w_{ij,mn} \hat{c}_i^\dagger \hat{c}_m^\dagger \hat{c}_k \hat{c}_n + \sum_{lk\alpha} V_{k\alpha,l}[\hat{c}_{k\alpha}^\dagger \hat{c}_l + \hat{c}_l^\dagger \hat{c}_{k\alpha}]. \qquad \text{(G.27)}$$

We need in the derivation following commutator relations

$$[\hat{c}_s, \hat{c}_l^\dagger \hat{c}_l] = \hat{c}_l \delta_{sl} \tag{G.28}$$

$$[\hat{c}_s, \hat{c}_i^\dagger \hat{c}_m^\dagger \hat{c}_i \hat{c}_n] = \hat{c}_m^\dagger \hat{c}_j \hat{c}_n \delta_{si} - \hat{c}_i^\dagger \hat{c}_j \hat{c}_n \delta_{sm}. \tag{G.29}$$

Calculatin the commutator $[\hat{c_s}(t), H]$ and multiplying by $\hat{c}_{l'}^\dagger(t')$ we obtain

$$i\partial_t \hat{c}_l(t)\hat{c}_{l'}^\dagger(t') = \varepsilon_l \hat{c}_l(t)\hat{c}_{l'}^\dagger(t') + \sum_{k\alpha} V_{k\alpha,l}\hat{c}_{k\alpha}(t)\hat{c}_{l'}^\dagger(t') + \sum_{jmn} w_{ij,mn}\hat{c}_m^\dagger \hat{c}_j(t)\hat{c}_n(t)\hat{c}_{l'}^\dagger(t'), \tag{G.30}$$

where by time-ordering and ensemble averaging we get an equation of motion for Green function $\mathbf{G}_{ll'}$

$$i\partial_t \mathbf{G}_{ll'}(t,t') = \varepsilon_l \mathbf{G}_{ll'}(t,t') + \sum_{k\alpha} V_{k\alpha l}\mathbf{G}_{k\alpha l'}(t,t') + \int_\gamma d\bar{t}\boldsymbol{\Sigma}_{ll''}(t,\bar{t})\mathbf{G}_{l''l'}(\bar{t},t') + \delta(t,t'). \tag{G.31}$$

Checking all the combinations we found following

$$\mathbf{G}_{ll'} = \mathbf{g}_l(t,t') + \sum_{k\alpha} V_{l,k\alpha} \int d\bar{t}\mathbf{g}_l(t,\bar{t})\mathbf{G}_{k\alpha,l}(\bar{t},t') + \int d\bar{t}\mathbf{g}_l(t,\bar{t})[\boldsymbol{\Sigma}\cdot G]_{ll'}(\bar{t},t') \tag{G.32}$$

$$\mathbf{G}_{lk\alpha} = \sum_{k\alpha'} V_{l,k\alpha} \int d\bar{t}\mathbf{g}_l(t,\bar{t})\mathbf{G}_{k\alpha,k'\alpha'}(\bar{t},t') \tag{G.33}$$

$$\mathbf{G}_{k\alpha,k\alpha} = \delta_{\alpha,\alpha'}\mathbf{g}_{k\alpha}(t,t') + \sum_l V_{k\alpha,l} \int d\bar{t}\mathbf{g}_{k\alpha}(t,\bar{t})\mathbf{G}_{l,k\alpha}(\bar{t},t') \tag{G.34}$$

$$\mathbf{G}_{k\alpha,l'} = \sum_l V_{k\alpha,l} \int dt\mathbf{g}_{k\alpha}(t,\bar{t})\mathbf{G}_{ll'}(\bar{t},t'). \tag{G.35}$$

Rewriting in the matrix from we have

$$\mathbf{G}_{cc} = \mathbf{g}_c(t,t') + \int d\bar{t}\mathbf{g}_c(t,\bar{t})V_{c\alpha}\mathbf{G}_{\alpha c}(\bar{t},t') + \int d\bar{t}\bar{\bar{t}}\mathbf{g}_c t,\bar{t}\boldsymbol{\Sigma}_{cc}(\bar{t},\bar{\bar{t}})\mathbf{G}_{cc}(\bar{\bar{t}},t') \tag{G.36}$$

$$\mathbf{G}_{\alpha c}(t,t') = \int d\bar{t}\mathbf{g}_\alpha(t,\bar{t})V_{\alpha c}\mathbf{G}_{cc}(t,t') \tag{G.37}$$

$$\mathbf{G}_{\alpha\alpha'}(t,t') = \delta_{\alpha\alpha'}\mathbf{g}_\alpha(t,t') + \int d\bar{t}\mathbf{g}_\alpha(t,\bar{t})V_{\alpha c}\mathbf{G}_{c\alpha'}(\bar{t},t') \tag{G.38}$$

$$\mathbf{G}_{c\alpha}(t,t') = \int d\bar{t}\mathbf{g}_c(t,\bar{t})V_{c\alpha}\mathbf{G}_{\alpha,\alpha'}(t,t'). \tag{G.39}$$

We could also have considered the commutator between the Hamiltonian and creation operator. This would have let us to obtain more expressions for different components of G.

G.3 Proof of equation (5.101)

Here the following equation is proved. The following statement is proved for the lesser function (the greater function is proved in a similar fashion)

$$\mathbf{G}^{\gtrless}(z,z') = \mathbf{G}^{R}(z,0)\mathbf{G}^{\gtrless}(0,0)\mathbf{G}^{A}(0,z') + \mathbf{\Delta}^{\gtrless}(z,z') \tag{G.40}$$

where ($\mathbf{G}^{K} \equiv \mathbf{G}^{>} + \mathbf{G}^{<}$)

$$\begin{aligned}\mathbf{\Delta}^{\gtrless}(z,z') = i\mathbf{G}^{R}(z,0)\mathbf{G}^{>}(0,z') - i\mathbf{G}^{<}(z,0)\mathbf{G}^{A}(0,z') - \mathbf{G}^{R}(z,0)\mathbf{G}^{K}(0,0)\mathbf{G}^{A}(0,z') \\ + \left[\mathbf{G}^{R}\cdot\left[\mathbf{\Sigma}^{\gtrless} + \mathbf{\Sigma}^{\rceil} * G * \mathbf{\Sigma}^{\lceil}\right]\cdot\mathbf{G}^{A}\right](z,z')\end{aligned} \tag{G.41}$$

The Green function can be expressed with help of some reference Green function $\mathbf{G}_0$, which is usually noninteracting Green function, as a Dyson equation

$$\mathbf{G}(z,z') = \mathbf{G}_0(z,z') + \int d\bar{z}d\bar{\bar{z}}\mathbf{G}_0(z,\bar{z})\mathbf{\Sigma}(\bar{z},\bar{\bar{z}})\mathbf{G}(\bar{\bar{z}},z) \tag{G.42}$$

The lesse component of the Green function can be obtained by using Langreth theorem

$$\begin{aligned}\mathbf{G}^{<}(z,z') &= \mathbf{G}_0^{<}(z,z') + \int_0^z d\bar{z}\mathbf{G}_0^{R}(z,\bar{z})[\mathbf{\Sigma}G]^{<}(\bar{z},z') \\ &+ \int_0^{z'} d\bar{z}\mathbf{G}_0^{<}[\mathbf{\Sigma}G]^{A} + \int_0^{-i\beta} d\tau\mathbf{G}_0^{\rceil}[\mathbf{\Sigma}G]^{\lceil} \\ &= \mathbf{G}_0^{<} + \mathbf{G}_0^{R}\cdot[\mathbf{\Sigma}G]^{<} + \mathbf{G}_0^{<}\cdot[\mathbf{\Sigma}G]^{A} + \mathbf{G}^{\rceil}\star[\mathbf{\Sigma}G]^{\lceil}\end{aligned} \tag{G.43}$$

using the Langreth theorem again to the terms $[\mathbf{\Sigma}G]^{\{<,A,\lceil\}}$ we get

$$\begin{aligned}\mathbf{G}^{<} = \mathbf{G}_0(\delta - \mathbf{G}_0\cdot\mathbf{\Sigma}^{R}\cdot\mathbf{G}^{A}) + \mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{R}\cdot\mathbf{G}^{<} + (\mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{<} + \mathbf{\Sigma}^{\rceil}\star\mathbf{\Sigma}^{\lceil})\cdot\mathbf{G}^{A} \\ +\mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{\rceil}\star\mathbf{G}^{\lceil} + \mathbf{G}^{\rceil}\star\mathbf{\Sigma}\star\mathbf{G}^{\lceil}\end{aligned} \tag{G.44}$$

This equation can be solved for $\mathbf{G}^{<}$. Writing first

$$\begin{aligned}(\delta + \mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{R})\mathbf{G}^{<} = \mathbf{G}_0(\delta - \mathbf{\Sigma}^{R}\cdot\mathbf{G}^{A}) + (\mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{<} + \mathbf{\Sigma}^{\rceil}\star\mathbf{\Sigma}^{\lceil})\cdot\mathbf{G}^{A} \\ +\mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{\rceil}\star\mathbf{G}^{\lceil} + \mathbf{G}^{\rceil}\star\mathbf{\Sigma}\star\mathbf{G}^{\lceil}\end{aligned} \tag{G.45}$$

Using the definition of the retarded Green functions $\mathbf{G}^{R}(z,z') = \theta(z-z')(\mathbf{G}^{>}(z,z') - \mathbf{G}^{<}(z,z'))$ the factor in front of $\mathbf{G}^{>}$ can be expressed as $(\delta - \mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{R})) = \mathbf{G}_0^{R}(\mathbf{G}^{R})^{-1}$. E.g.

$$\begin{aligned}\mathbf{G}^{>} - \mathbf{G}^{<} &= (\mathbf{G}_0^{>} - \mathbf{G}_0^{<})(\delta + \mathbf{\Sigma}^{A}\cdot\mathbf{G}^{A}) + \mathbf{G}_0^{R}\cdot\mathbf{\Sigma}^{R}\cdot\mathbf{G}^{<} + \mathbf{G}_0^{R}\mathbf{\Sigma}^{<}\mathbf{G}^{A} \\ &= \mathbf{G}_0^{R}(\delta + \mathbf{\Sigma}^{R}\mathbf{G}^{R})\end{aligned} \tag{G.46}$$

Then we have

$$\begin{aligned}\mathbf{G}_0^R(\mathbf{G}^R)^{-1}\mathbf{G}^< = \mathbf{G}_0(\delta - \mathbf{G}_0\cdot\mathbf{\Sigma}^R\cdot\mathbf{G}^A) + (\mathbf{G}_0^R\cdot\mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil\star\mathbf{\Sigma}^\lceil)\cdot\mathbf{G}^A \\ +\mathbf{G}_0^R\cdot\mathbf{\Sigma}^\rceil\star\mathbf{G}^\lceil + \mathbf{G}^\rceil\star\mathbf{\Sigma}\star\mathbf{G}^\lceil.\end{aligned} \tag{G.47}$$

Multiplying this equation from the right with $(\mathbf{G}_0^R)^-1\mathbf{G}^R$ which is according to Dyson equation same as $\delta + \mathbf{\Sigma}^R\mathbf{G}^R$ we get

$$\begin{aligned}\mathbf{G}^< = (\delta + \mathbf{\Sigma}^R\mathbf{G}^R)\mathbf{G}_0^<(\delta - \mathbf{\Sigma}^R\cdot\mathbf{G}^A) + (\delta + \mathbf{\Sigma}^R\mathbf{G}^R)(\mathbf{G}_0^R\cdot\mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil\star\mathbf{\Sigma}^\lceil)\cdot\mathbf{G}^A \\ +(\delta + \mathbf{\Sigma}^R\mathbf{G}^R)(\mathbf{G}_0^R\cdot\mathbf{\Sigma}^\rceil\star\mathbf{G}^\lceil + \mathbf{G}^\rceil\star\mathbf{\Sigma}\star\mathbf{G}^\lceil).\end{aligned} \tag{G.48}$$

Using following identities this equation can be simplified further

$$\mathbf{G}_0^{\gtrless}(t,t') = \mathbf{G}_0^R(t,0)\mathbf{G}_0^{\gtrless}(0,0)\mathbf{G}_0^A(0,t') \tag{G.49}$$

$$\mathbf{G}_0(\tau,t) = -i\mathbf{G}_0(\tau,0)\mathbf{G}_0^A(0,t) \tag{G.50}$$

$$\mathbf{G}_0(t,\tau) = i\mathbf{G}_0^R(t,0)\mathbf{G}_0(0,\tau) \tag{G.51}$$

we get

$$\mathbf{G}^< = \mathbf{G}^R(z,0)\mathbf{G}^<(0,0)\mathbf{G}^A(0,z). \tag{G.52}$$

Using the Dyson equation for $\mathbf{G}(t,\tau)$ and for $\mathbf{G}(\tau,\tau')$

$$\mathbf{G}(\tau,\tau') = \mathbf{G}_0(\tau,\tau') + [\mathbf{G}_0\star\mathbf{\Sigma}\star G](\tau,\tau') \tag{G.53}$$

$$\mathbf{G}(\tau,t) = [\mathbf{G}^R\cdot\mathbf{\Sigma}^\rceil\star G](\tau,t) + i\mathbf{G}^R(t,0)\mathbf{G}(0,\tau) \tag{G.54}$$

$$\mathbf{G}(t,\tau) = [G\star\mathbf{\Sigma}^\lceil\cdot\mathbf{G}^A](t,\tau) - i\mathbf{G}(\tau,0)\mathbf{G}^A(0,t) \tag{G.55}$$

we end up to an equation

$$\begin{aligned}\mathbf{G}^< = \mathbf{G}^R\cdot G\cdot\mathbf{G}^A + \mathbf{G}^R\cdot[\mathbf{\Sigma}^< + \mathbf{\Sigma}^\rceil\star G\star\mathbf{\Sigma}^\lceil](z,z') \\ +i\mathbf{G}^R(z,0)[G\star\mathbf{\Sigma}^\lceil\cdot\mathbf{G}^A](0,z') - i[\mathbf{G}^R\cdot\mathbf{\Sigma}^\lceil\star G](z,0)\mathbf{G}^A(0,z')\end{aligned} \tag{G.56}$$

with help of the Dyson equations we can write the last two terms as

$$i\mathbf{G}^R(z,0)[G\star\mathbf{\Sigma}^\lceil\cdot\mathbf{G}^A](0,z' = i\mathbf{G}^R(z,0)\mathbf{G}^>(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^>(0,0)\mathbf{G}^A(0,z') \tag{G.57}$$

and

$$-i[\mathbf{G}^R\cdot\mathbf{\Sigma}^\lceil\star G](z,0)\mathbf{G}^A(0,z') = -i\mathbf{G}^<(z,0)\mathbf{G}^A(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^<(0,0)\mathbf{G}^A(0,z'). \tag{G.58}$$

This leads us to the final result

$$\begin{aligned}\mathbf{G}^{\gtrless}(z,z') = \mathbf{G}^R(z,0)\mathbf{G}^{\gtrless}(0,0)\mathbf{G}^A(0,z') + i\mathbf{G}^R(z,0)\mathbf{G}^>(0,z') \\ i\mathbf{G}^<(z,0)\mathbf{G}^A(0,z') - \mathbf{G}^R(z,0)\mathbf{G}^K(0,0)\mathbf{G}^A(0,z') \\ + \left[\mathbf{G}^R\cdot\left[\mathbf{\Sigma}^{\gtrless} + \mathbf{\Sigma}^\rceil * G * \mathbf{\Sigma}^\lceil\right]\cdot\mathbf{G}^A\right](z,z').\end{aligned} \tag{G.59}$$

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