

# An Introduction to Nonequilibrium Green Functions

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# Chapter 1

## Introduction

### 1.1 Why nonequilibrium Green functions ?

In these lectures notes we discuss a method that is not very familiar to most quantum chemists, the nonequilibrium Green function method. However, this is likely to change mainly due to new developments in nanoscience and the emerging field of 'molecular electronics' in which single molecules are used as conducting elements attached to electrodes. Description of such situations is a challenge for the theorist as it requires a description fast time-dependent processes in strong external fields. The traditional quantum chemistry approaches that take into account electron correlations in stationary systems can not deal with these situations. This has been our main reason for looking at the nonequilibrium Green function method, which has had important applications within solid state, nuclear and plasma physics. However, due to its general nature it can equally deal with molecular systems. Let us briefly describe its main features:

- The method has as its main ingredient the Green function, which is a function of two space-time coordinates. From knowledge of this function one can calculate time-dependent expectation values such as currents and densities, electron addition and removal energies and the total energy of the system.
- In the absence of external fields the nonequilibrium Green function method reduces to the equilibrium Green function method which has had important applications in quantum chemistry.
- Nonequilibrium Green functions can be applied to both extended and finite systems.
- The nonequilibrium Green function can handle strong external fields nonperturbatively. The electron-electron interactions are taken into account by infinite summations.
- The approximations within the nonequilibrium Green function method can be chosen such that macroscopic conservation laws as those of particle number, momentum and angular momentum are automatically satisfied

- Dissipative processes and memory effects in transport that occur due to electron-electron interactions and coupling of electronic to nuclear vibrations can be clearly diagrammatically analyzed

## 1.2 References

Many more things can be said about nonequilibrium Green functions. We therefore give a list of references for further reading that we found useful ourselves:

### Nonequilibrium Green functions

- P.Danielewicz, *Quantum Theory of Nonequilibrium Processes*, Annals of Physics, **152**, 239, (1984)
- H.Haug and A.-P.Jauho, *Quantum Kinetics in Transport and Optics of Semi-conductors*, Springer-Verlag, Berlin (1998)
- L.P.Kadanoff and G.Baym, *Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems*, Addison-Wesley, (1989)
- M.Bonitz, *Quantum Kinetic Theory*, Teubner, Stuttgart-Leipzig, (1998)
- J.Rammer and H.Smith, *Quantum field-theoretical methods in transport theory of metals*, Rev.Mod.Phys. **58**, (1986)
- G.Stefanucci and C.-O.Almbladh, *Time-dependent partition-free approach in resonant tunneling systems*, Phys.Rev.B**69**, 195318 (2004)

### Equilibrium Green function theory

- E.K.U.Gross, E.Runge and O.Heinonen, *Many-Particle Theory*, Adam-Hilger, Bristol (1991)
- A.L.Fetter and J.D.Walecka, *Quantum Theory of Many-Particle Systems*, Dover, (2003)
- L.Hedin and S.Lundqvist, *Effects of electron-electron and electron-phonon interactions on the one-electron states of solids*, Solid State Physics **23**, 1969
- J.Linderberg and Y.Öhrn, *Propagators in Quantum Chemistry*, Wiley-Interscience, (2004)

## Chapter 2

# Second quantization

### 2.1 The Schrödinger equation

The goal of these lectures notes is to describe many-electron systems in general time-dependent external fields. We will restrict ourselves to a nonrelativistic description and therefore we restrict ourselves to a discussion of the time-dependent Schrödinger equation (TDSE). The TDSE of  $n$ -particles has the form

$$(i\partial_t - \hat{H}(t))\Psi(\mathbf{x}_1, \dots, \mathbf{x}_n, t) = 0 \quad (2.1)$$

where  $\mathbf{x}_i = \mathbf{r}_i\sigma_i$  denotes a space-spin variable of particle  $i$ . Now the Hamiltonian is invariant under interchange of two particles. This implies that the eigenstates of the Hamiltonian can be chosen to transform according to an irreducible representation of the permutation group. Experience teaches us that only the one-dimensional representations, i.e. the completely symmetric or completely anti-symmetric representations seem to occur in nature. If this assumption is made, a famous theorem of Pauli states that the symmetric representation necessarily describes particles with integer spin whereas the anti-symmetric representation necessarily describes particle with half-integer spin. The proof is based on the properties of the representations of the Lorentz group and is therefore an essentially relativistic result. It would go too far to describe this in detail and we simply use the result. Since electrons are spin-half particles they are described by anti-symmetric wave functions:

$$\Psi(\dots \mathbf{x}_i \dots \mathbf{x}_j \dots) = -\Psi(\dots \mathbf{x}_j \dots \mathbf{x}_i \dots) \quad (2.2)$$

In the following section we will introduce a formalism that will automatically take this symmetry into account within the operators. This formalism is commonly known as second quantization and is used in most advanced many-body approaches. Knowledge of this formalism is therefore essential to understand a great number of research papers.

## 2.2 Fock space and field operators

### 2.2.1 Definitions

In this section we will define a space, the so-called Fock space, of quantum states that consist of linear combinations of states with different number of particles. There are several reasons for doing this.

- This will provide us with a natural framework to discuss processes that change the number of particles, such as in ionization.
- It will allow us to consider temperature dependent systems and calculate expectation values within the grand canonical ensemble in which the particle number is not fixed.
- By dealing with creation and annihilation operators in Fock space the anti-symmetry properties of the wavefunctions are automatically built into the anti-commutation relations of the operators and we never have to deal with the wavefunctions themselves.

Let  $\{|\Psi_{j,N}\rangle\}$  be a complete set of states in a  $N$ -particle Hilbert space. Then Fock space is defined as the set of linear combinations of the form

$$|F\rangle = \alpha_0|0\rangle + \sum_{N=1}^{\infty} \sum_{j=1}^{\infty} \alpha_j^N |\Psi_{j,N}\rangle \quad (2.3)$$

The zero-particle Hilbert space is one-dimensional and has only one basis function  $|0\rangle$  which can be identified with the number 1. Let

$$|G\rangle = \beta_0|0\rangle + \sum_{N=1}^{\infty} \sum_{j=1}^{\infty} \beta_j^N |\Phi_{j,N}\rangle \quad (2.4)$$

be another element of Fock space with respect to some other basis  $\{|\Phi_{j,N}\rangle\}$  then the inner product is defined as

$$\langle F|G\rangle \equiv \alpha_0^* \beta_0 + \sum_{N=1}^{\infty} \sum_{i,j=1}^{\infty} \alpha_j^{N*} \beta_i^N \langle \Psi_{j,N} | \Phi_{i,N} \rangle \quad (2.5)$$

where  $\langle \Psi_{j,N} | \Phi_{i,N} \rangle$  is the inner product in  $N$ -particle Hilbert space. One can check that definition Eq.(2.5) satisfies all the usual requirements of an inner product. We also see that according to our definition the Fock overlap between states containing different number of particles is zero, i.e. if  $|F\rangle = |\Psi_{i,N}\rangle$  and  $|G\rangle = |\Phi_{j,M}\rangle$  then  $\langle F|G\rangle = 0$  when  $N \neq M$ . Since we will only consider fermions we further assume that all the  $N$ -particle Hilbert spaces consist of anti-symmetric functions.

We are now ready to define the annihilation and creation operators that map wavefunctions from an  $n$ -particle Hilbert space to, respectively a  $n - 1$  and a  $n + 1$ -particle Hilbert space. We define the action of the annihilation operator  $\hat{\psi}(\mathbf{x})$  as

$$(\hat{\psi}(\mathbf{x})\Psi_n)(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}) \equiv \sqrt{n} \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}) \quad (2.6)$$



This operator maps an  $n$ -particle state to a  $n - 1$  particle state. If  $\Psi_n$  is anti-symmetric it is not difficult to see that the resulting  $n - 1$ -particle state is again anti-symmetric. Corresponding to this annihilation operator  $\hat{\psi}(\mathbf{x})$  we define the adjoint operator  $\hat{\psi}^\dagger(\mathbf{x})$  which maps a  $n$ -particle state to a  $n + 1$ -particle state. This operator is called the creation operator. The explicit action of this operator on a  $n$ -particle state  $\Psi_n$  is

$$(\hat{\psi}^\dagger(\mathbf{x})\Psi_n)(\mathbf{x}_1, \dots, \mathbf{x}_{n+1}) \equiv \frac{(-1)^n}{\sqrt{n+1}} \sum_{j=1}^{n+1} (-1)^{j+1} \delta(\mathbf{x} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \hat{\mathbf{x}}_j \dots \mathbf{x}_{n+1}) \quad (2.7)$$

where  $\hat{\mathbf{x}}_j$  denotes that this argument is lacking. For example  $(\mathbf{x}_1, \hat{\mathbf{x}}_2, \mathbf{x}_3, \mathbf{x}_4) = (\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4)$ . Let us check that  $\hat{\psi}^\dagger$  is indeed the adjoint of  $\hat{\psi}$ . We have

$$\langle \Phi_{n-1} | \hat{\psi}(\mathbf{x}) | \Psi_n \rangle = \sqrt{n} \int d\mathbf{x}_1 \dots d\mathbf{x}_{n-1} \Phi_{n-1}^*(\mathbf{x}_1 \dots \mathbf{x}_{n-1}) \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{n-1}, \mathbf{x}) \quad (2.8)$$

On the other hand we also have

$$\begin{aligned} \langle \Psi_n | \hat{\psi}^\dagger(\mathbf{x}) | \Phi_{n-1} \rangle^* &= \frac{1}{\sqrt{n}} (-1)^{n-1} \sum_{j=1}^n (-1)^{j+1} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_n) \\ &\quad \times \delta(\mathbf{x} - \mathbf{x}_j) \Phi_{n-1}^*(\mathbf{x}_1 \dots \hat{\mathbf{x}}_j \dots \mathbf{x}_n) \\ &= \frac{1}{\sqrt{n}} (-1)^{n-1} \sum_{j=1}^n (-1)^{j+1} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1} \dots \mathbf{x}_n) \\ &\quad \times \Phi_{n-1}^*(\mathbf{x}_1 \dots \hat{\mathbf{x}}_j \dots \mathbf{x}_n) \\ &= \frac{1}{\sqrt{n}} (-1)^{n-1} \sum_{j=1}^n (-1)^{j+1} (-1)^{n-j} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{j-1}, \mathbf{x}_{j+1} \dots \mathbf{x}_n, \mathbf{x}) \\ &\quad \times \Phi_{n-1}^*(\mathbf{x}_1 \dots \mathbf{x}_{j-1}, \mathbf{x}_{j+1} \dots \mathbf{x}_n) \\ &= \frac{1}{\sqrt{n}} \sum_{j=1}^n \int d\mathbf{x}_1 \dots d\mathbf{x}_{n-1} \Phi_{n-1}^*(\mathbf{x}_1 \dots \mathbf{x}_{n-1}) \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{n-1}, \mathbf{x}) \\ &= \sqrt{n} \int d\mathbf{x}_1 \dots d\mathbf{x}_{n-1} \Phi_{n-1}^*(\mathbf{x}_1 \dots \mathbf{x}_{n-1}) \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{n-1}, \mathbf{x}) \end{aligned} \quad (2.9)$$

From Eqns.(2.8) and (2.9) we see that

$$\langle \Phi_{n-1} | \hat{\psi}(\mathbf{x}) | \Psi_n \rangle = \langle \Psi_n | \hat{\psi}^\dagger(\mathbf{x}) | \Phi_{n-1} \rangle^* \quad (2.10)$$

From this result it is simple to prove that for any Fock space states  $F$  and  $G$  we have

$$\langle F | \hat{\psi}(\mathbf{x}) | G \rangle = \langle G | \hat{\psi}^\dagger(\mathbf{x}) | F \rangle^* \quad (2.11)$$

This proves that  $\hat{\psi}^\dagger(\mathbf{x})$  is the adjoint of  $\hat{\psi}(\mathbf{x})$ .

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### Exercise

Prove relation (2.11) from Eq.(2.10)

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We did not check sofar that  $\hat{\psi}^\dagger(\mathbf{x})|\Psi_n\rangle$  is indeed an anti-symmetric  $n + 1$ -particle state if  $\Psi_n$  is antisymmetric. However, this is readily checked as well. Let us interchange elements  $p$  and  $q$  with  $p > q$ . Then we first write

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x})|\Psi_n\rangle &= \frac{(-1)^n}{\sqrt{n+1}} \sum_{j=1(j \neq p, q)}^{n+1} (-1)^{j+1} \delta(\mathbf{x} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \hat{\mathbf{x}}_j \dots \mathbf{x}_{n+1}) \\
&+ \frac{(-1)^n}{\sqrt{n+1}} (-1)^p \Psi(\mathbf{x}_1 \dots \hat{\mathbf{x}}_p \dots \mathbf{x}_{n+1}) \\
&+ \frac{(-1)^n}{\sqrt{n+1}} (-1)^q \Psi(\mathbf{x}_1 \dots \hat{\mathbf{x}}_q \dots \mathbf{x}_{n+1})
\end{aligned} \tag{2.12}$$

The first term in this equation is certainly anti-symmetric if we interchange  $p$  and  $q$ . Let us therefore consider the last two terms. Interchanging  $\mathbf{x}_p$  and  $\mathbf{x}_q$  for these terms gives

$$\begin{aligned}
&(-1)^p \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{q-1}, \mathbf{x}_p, \mathbf{x}_{q+1} \dots \hat{\mathbf{x}}_p \dots \mathbf{x}_{n+1}) + (-1)^p \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_q, \dots \mathbf{x}_{p-1}, \mathbf{x}_q, \mathbf{x}_{p+1} \dots \mathbf{x}_{n+1}) \\
&= (-1)^p (-1)^{p-q+1} \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_q \dots \mathbf{x}_{n+1}) + (-1)^q (-1)^{p-q+1} \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_p \dots \mathbf{x}_{n+1}) \\
&= -(-1)^q \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_q \dots \mathbf{x}_{n+1}) - (-1)^p \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_p \dots \mathbf{x}_{n+1})
\end{aligned} \tag{2.13}$$

which indeed yields an overall minus sign. We thus see that the creation operator maps an anti-symmetric  $n$ -particle state to an anti-symmetric  $n + 1$ -particle state.

## 2.2.2 Anti-commutation relations

We subsequently prove a basic anti-commutation relation satisfied by the field operators. We calculate

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}')\Psi_n &= \hat{\psi}^\dagger(\mathbf{x})\sqrt{n}\Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}') \\
&= (-1)^{n-1} \sum_{j=1}^n (-1)^{j+1} \delta(\mathbf{x} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_j \dots \mathbf{x}_n, \mathbf{x}') \\
&= (-1)^{n-1} \sum_{j=1}^n (-1)^{j+1} \delta(\mathbf{x} - \mathbf{x}_j) (-1)^{n-j} \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}', \mathbf{x}_j \dots \mathbf{x}_n) \\
&= \sum_{j=1}^n \delta(\mathbf{x} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}', \mathbf{x}_j \dots \mathbf{x}_n)
\end{aligned} \tag{2.14}$$

We further have

$$\begin{aligned}
\hat{\psi}(\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x})\Psi_n &= \hat{\psi}(\mathbf{x}')\frac{1}{\sqrt{n+1}}(-1)^n\sum_{j=1}^{n+1}(-1)^{j+1}\delta(\mathbf{x}-\mathbf{x}_j)\Psi_n(\mathbf{x}_1,\dots,\hat{\mathbf{x}}_j,\dots,\mathbf{x}_{n+1}) \\
&= (-1)^n\sum_{j=1}^n(-1)^{j+1}\delta(\mathbf{x}-\mathbf{x}_j)\Psi_n(\mathbf{x}_1,\dots,\hat{\mathbf{x}}_j,\dots,\mathbf{x}_n,\mathbf{x}') \\
&\quad + (-1)^n(-1)^{n+2}\delta(\mathbf{x}-\mathbf{x}')\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_n) \\
&= (-1)^n\sum_{j=1}^n(-1)^{j+1}(-1)^{n-j}\delta(\mathbf{x}-\mathbf{x}_j)\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_{j-1},\mathbf{x}',\mathbf{x}_{j+1},\dots,\mathbf{x}_n) \\
&\quad + \delta(\mathbf{x}-\mathbf{x}')\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_n) \\
&= -\sum_{j=1}^n\delta(\mathbf{x}-\mathbf{x}_j)\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_{j-1},\mathbf{x}',\mathbf{x}_{j+1},\dots,\mathbf{x}_n) \\
&\quad + \delta(\mathbf{x}-\mathbf{x}')\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_n)
\end{aligned} \tag{2.15}$$

From Eqns.(2.14) and (2.15) we find

$$\left[\hat{\psi}(\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x}) + \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}')\right]\Psi_n = \delta(\mathbf{x}-\mathbf{x}')\Psi_n \tag{2.16}$$

for any wave function  $\Psi_n$ . We thus obtain the basic anti-commutation relation for the field operators

$$\left\{\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}(\mathbf{x}')\right\} = \delta(\mathbf{x}-\mathbf{x}') \tag{2.17}$$

where anti-commutation brackets are defined as

$$\left\{\hat{A}, \hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A} \tag{2.18}$$

Further anti-commutation between the field operators are readily derived. We have

$$\begin{aligned}
\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}')\Psi_n &= \sqrt{n}\sqrt{n-1}\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_{n-2},\mathbf{x},\mathbf{x}') \\
&= -\sqrt{n}\sqrt{n-1}\Psi_n(\mathbf{x}_1,\dots,\mathbf{x}_{n-2},\mathbf{x}',\mathbf{x}) \\
&= -\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})\Psi_n
\end{aligned} \tag{2.19}$$

for any  $\Psi_n$  and therefore we have

$$\left\{\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')\right\} = 0 \tag{2.20}$$

By taking the adjoint of this relation we then immediately also have

$$\left\{\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right\} = 0 \tag{2.21}$$

## 2.3 The Hamiltonian in second quantization

With the relation derived in the previous section it is not difficult to express the Hamiltonian in terms of field operators. Any one-body multiplicative or differential operator  $\hat{O}$  can be written as

$$\hat{O} = \sum_i o(\mathbf{x}_i) = \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x})o(\mathbf{x})\hat{\psi}(\mathbf{x}) \tag{2.22}$$

*Proof.* Using Eq.(2.14) we have

$$\begin{aligned}
\int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) o(\mathbf{x}) \hat{\psi}(\mathbf{x}) |\Psi_n\rangle &= \int d\mathbf{x} o(\mathbf{x}') \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}') \Big|_{\mathbf{x}'=\mathbf{x}} |\Psi_n\rangle \\
&= \sum_j \int d\mathbf{x} o(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{j-1}, \mathbf{x}', \mathbf{x}_{j+1} \dots \mathbf{x}_n) \Big|_{\mathbf{x}'=\mathbf{x}} \\
&= \sum_j o(\mathbf{x}_j) |\Psi_n\rangle
\end{aligned} \tag{2.23}$$

For example for the second quantized expressions for the kinetic energy and a time-dependent external scalar potential are given by

$$\begin{aligned}
\hat{T} &= \sum_i -\frac{1}{2} \nabla_i^2 = -\frac{1}{2} \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \nabla^2 \hat{\psi}(\mathbf{x}) \\
\hat{V}(t) &= \sum_i v(\mathbf{x}_i t) = \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) v(\mathbf{x}, t)
\end{aligned} \tag{2.24}$$

Another example, is, for instance, the density operator

$$\hat{n}(\mathbf{y}) = \sum_i \delta(\mathbf{y} - \mathbf{x}_i) = \int d\mathbf{x} \delta(\mathbf{y} - \mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}) \tag{2.25}$$

We can further consider two-body operators. Let us consider the expression

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x}) |\Psi_n\rangle &= \sqrt{n} \sqrt{n-1} \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{y}, \mathbf{x}) \\
&= \sqrt{n} (-1)^{n-2} \hat{\psi}^\dagger(\mathbf{x}) \sum_{j=1}^{n-1} (-1)^{j+1} \delta(\mathbf{y} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \hat{\mathbf{x}}_j, \dots, \mathbf{x}_{n-1}, \mathbf{y}, \mathbf{x}) \\
&= \sqrt{n} (-1)^n \hat{\psi}^\dagger(\mathbf{x}) \sum_j^{n-1} (-1)^{j+1} (-1)^{n-1-j} \delta(\mathbf{y} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}) \\
&= \sqrt{n} \hat{\psi}^\dagger(\mathbf{x}) \Phi_{n-1}^{(\mathbf{x}, \mathbf{y})}(\mathbf{x}_1 \dots \mathbf{x}_{n-1})
\end{aligned} \tag{2.26}$$

where we defined the wavefunction

$$\Phi_{n-1}^{(\mathbf{x}, \mathbf{y})}(\mathbf{x}_1 \dots \mathbf{x}_{n-1}) = [\delta(\mathbf{y} - \mathbf{x}_1) + \dots + \delta(\mathbf{y} - \mathbf{x}_n)] \Psi_n(\mathbf{x}_1 \dots \mathbf{x}_{n-1}, \mathbf{x}) \tag{2.27}$$

Now since

$$\begin{aligned}
\Phi_{n-1}^{(\mathbf{x}, \mathbf{y})}(\mathbf{x}_1 \dots \hat{\mathbf{x}}_k \dots \mathbf{x}_n) &= \sum_{j=1(j \neq k)}^n \delta(\mathbf{y} - \mathbf{x}_j) \Phi_n(\mathbf{x}_1 \dots \hat{\mathbf{x}}_k \dots, \mathbf{x}_n, \mathbf{x}) \\
&= (-1)^{n-k} \sum_{j=1(j \neq k)}^n \delta(\mathbf{y} - \mathbf{x}_j) \Phi_n(\mathbf{x}_1 \dots \mathbf{x}_{k-1}, \mathbf{x}, \mathbf{x}_{k+1} \dots, \mathbf{x}_n)
\end{aligned} \tag{2.28}$$

it follows from Eq.(2.26) and Eq.(2.28) that

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x}) |\Psi_n\rangle &= \sqrt{n} \hat{\psi}^\dagger(\mathbf{x}) \Phi_{n-1}^{(\mathbf{x}, \mathbf{y})}(\mathbf{x}_1 \dots \mathbf{x}_{n-1}) \\
&= (-1)^{n-1} \sum_k^n (-1)^{k+1} \delta(\mathbf{x} - \mathbf{x}_k) \Phi_{n-1}^{(\mathbf{x}, \mathbf{y})}(\mathbf{x}_1 \dots \hat{\mathbf{x}}_k \dots \mathbf{x}_n) \\
&= \sum_{i,j(i \neq j)}^n \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{y} - \mathbf{x}_j) \Psi_n(\mathbf{x}_1, \dots, \mathbf{x}_n)
\end{aligned} \tag{2.29}$$

So we derived the expression

$$\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) = \sum_{j \neq k}^n \delta(\mathbf{x} - \mathbf{x}_k)\delta(\mathbf{y} - \mathbf{x}_j) \quad (2.30)$$

We see that for the two-particle interaction we can write

$$\begin{aligned} \hat{W} &= \frac{1}{2} \sum_{j \neq k}^n w(\mathbf{x}_j, \mathbf{x}_k) = \frac{1}{2} \int d\mathbf{x}d\mathbf{y} w(\mathbf{x}, \mathbf{y}) \sum_{j \neq k}^n \delta(\mathbf{x} - \mathbf{x}_k)\delta(\mathbf{y} - \mathbf{x}_j) \\ &= \frac{1}{2} \int d\mathbf{x}d\mathbf{y} w(\mathbf{x}, \mathbf{y}) \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \end{aligned} \quad (2.31)$$

Therefore a general Hamiltonian of the form

$$\hat{H}(t) = \sum_{j=1}^n h(\mathbf{x}_j, t) + \frac{1}{2} \sum_{j \neq k}^n w(\mathbf{x}_j, \mathbf{x}_k) \quad (2.32)$$

can in terms of the field operators be written as

$$\hat{H}(t) = \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x})h(\mathbf{x}, t)\hat{\psi}(\mathbf{x}) + \frac{1}{2} \int d\mathbf{x}d\mathbf{y} w(\mathbf{x}, \mathbf{y}) \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \quad (2.33)$$

This is the main result of this section. Let further derive some other often used representation of the Hamiltonian. Let  $\varphi_i(\mathbf{x})$  be a complete set of orthonormal orbitals in a one-particle Hilbert space, i.e. we have

$$\delta_{ij} = \int d\mathbf{x} \varphi_i^*(\mathbf{x})\varphi_j(\mathbf{x}) \quad (2.34)$$

$$\delta(\mathbf{x} - \mathbf{y}) = \sum_{i=1}^{\infty} \varphi_i^*(\mathbf{x})\varphi_i(\mathbf{y}) \quad (2.35)$$

Then we can define the annihilation and creation operators with respect to this basis as

$$\hat{a}_i \equiv \int d\mathbf{x} \varphi_i^*(\mathbf{x}) \hat{\psi}(\mathbf{x}) \quad (2.36)$$

$$\hat{a}_i^\dagger \equiv \int d\mathbf{x} \varphi_i(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \quad (2.37)$$

From the properties of the complete set of orbitals and the anti-commutation relations of the field operators we then immediately find the expressions

$$\hat{\psi}(\mathbf{x}) = \sum_{i=1}^{\infty} \varphi_i(\mathbf{x}) \hat{a}_i \quad (2.38)$$

$$\hat{\psi}^\dagger(\mathbf{x}) = \sum_{i=1}^{\infty} \varphi_i^*(\mathbf{x}) \hat{a}_i^\dagger \quad (2.39)$$

$$\delta_{ij} = \{\hat{a}_i^\dagger, \hat{a}_j\} \quad (2.40)$$

$$0 = \{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} \quad (2.41)$$

---

**Exercise**

How do the operators  $\hat{a}_i$  and  $\hat{a}_i^\dagger$  act on a n-particle wavefunction? Derive expressions Eq.(2.38) to (2.40).

---

In terms of the operators  $\hat{a}_i$  and  $\hat{a}_i^\dagger$  the Hamiltonian the attains the following form

$$\hat{H}(t) = \sum_{i,j} h_{ij}(t) \hat{a}_i^\dagger \hat{a}_j + \sum_{i,j,k,l} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \quad (2.42)$$

where we defined the coefficients

$$h_{ij}(t) = \int d\mathbf{x} \varphi_i^*(\mathbf{x}) h(\mathbf{x}, t) \varphi_j(\mathbf{x}) \quad (2.43)$$

$$V_{ijkl} = \frac{1}{2} \int d\mathbf{x} d\mathbf{y} \varphi_i^*(\mathbf{x}) \varphi_j^*(\mathbf{y}) w(\mathbf{x}, \mathbf{y}) \varphi_k(\mathbf{y}) \varphi_l(\mathbf{x}) \quad (2.44)$$

---

**Exercise**

Derive the form of the Hamiltonian in Eq.(2.42).

---

### 2.3.1 Some useful relations

Finally we will derive some useful relations that play a role when we will discuss the equations of motion for the Green function later on. These relations are derived with straightforward use of the anti-commutation relations of the field operators. Let us evaluate the commutator

$$\begin{aligned} [\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{z})] &= \hat{\psi}(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{z}) - \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{z}) \hat{\psi}(\mathbf{x}) \\ &= \left[ \delta(\mathbf{x} - \mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{x}) \right] \hat{\psi}(\mathbf{z}) - \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{z}) \hat{\psi}(\mathbf{x}) \\ &= \delta(\mathbf{x} - \mathbf{y}) \hat{\psi}(\mathbf{z}) - \hat{\psi}^\dagger(\mathbf{y}) \left\{ \hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{z}) \right\} \\ &= \delta(\mathbf{x} - \mathbf{y}) \hat{\psi}(\mathbf{z}) \end{aligned} \quad (2.45)$$

Let  $\hat{O}$  now be a one-body operator. Then we immediately see from Eq.(2.45) that

$$\begin{aligned} [\hat{\psi}(\mathbf{x}), \hat{O}] &= [\hat{\psi}(\mathbf{x}), \int d\mathbf{y} \hat{\psi}^\dagger(\mathbf{y}) o(\mathbf{y}) \hat{\psi}(\mathbf{y})] = \int d\mathbf{y} o(\mathbf{z}) [\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{z})] \Big|_{\mathbf{z}=\mathbf{y}} \\ &= \int d\mathbf{y} o(\mathbf{z}) \delta(\mathbf{x} - \mathbf{y}) \hat{\psi}(\mathbf{z}) \Big|_{\mathbf{z}=\mathbf{y}} = o(\mathbf{x}) \hat{\psi}(\mathbf{x}) \end{aligned} \quad (2.46)$$

This was our first useful relation. Let us continue with the commutator of a two-body operator:

$$\begin{aligned}
[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})] &= \hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \\
&= \left[ \delta(\mathbf{x} - \mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{x}) \right] \hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \\
&= \delta(\mathbf{x} - \mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y}) \left( [\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})] + \hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{x}) \right) \hat{\psi}(\mathbf{y}) \\
&\quad - \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \\
&= \delta(\mathbf{x} - \mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) - \delta(\mathbf{x} - \mathbf{z})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) - \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z}) \left\{ \hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y}) \right\} \\
&= \delta(\mathbf{x} - \mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) + \delta(\mathbf{x} - \mathbf{z})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{z}) \tag{2.47}
\end{aligned}$$

With this relation we see immediately that the commutator of the field operator  $\hat{\psi}(\mathbf{x})$  with the two-particle interaction  $\hat{W}$  is given by

$$\begin{aligned}
[\hat{\psi}(\mathbf{x}), \hat{W}] &= \frac{1}{2} \int d\mathbf{y} d\mathbf{z} w(\mathbf{y}, \mathbf{z}) [\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})] \\
&= \frac{1}{2} \int d\mathbf{y} d\mathbf{z} w(\mathbf{y}, \mathbf{z}) \left( \delta(\mathbf{x} - \mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y}) + \delta(\mathbf{x} - \mathbf{z})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{z}) \right) \\
&= \int d\mathbf{z} w(\mathbf{x}, \mathbf{z})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{x}) \tag{2.48}
\end{aligned}$$

This is our second useful relation.

---

### Exercise

Derive analogously the following relations

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{z})] = -\delta(\mathbf{x} - \mathbf{z})\hat{\psi}^\dagger(\mathbf{y}) \tag{2.49}$$

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z})\hat{\psi}(\mathbf{y})] = -\delta(\mathbf{x} - \mathbf{y})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z}) - \delta(\mathbf{x} - \mathbf{z})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y}) \tag{2.50}$$

and consequently the following expressions for the commutator with a one-body operator  $\hat{O}$  and two-particle interaction  $\hat{W}$ :

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{O}] = -o(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}) \tag{2.51}$$

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{W}] = - \int d\mathbf{z} w(\mathbf{x}, \mathbf{z})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{z})\hat{\psi}(\mathbf{z}) \tag{2.52}$$

---

We now collect our results and calculate the commutator of the field operators with the Hamiltonian. We the relations derived above we obtain:

$$[\hat{\psi}(\mathbf{x}), \hat{H}(t)] = h(\mathbf{x}, t)\hat{\psi}(\mathbf{x}) + \int d\mathbf{y} w(\mathbf{x}, \mathbf{y})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \tag{2.53}$$

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{H}(t)] = -h(\mathbf{x}, t)\hat{\psi}^\dagger(\mathbf{x}) - \int d\mathbf{y} w(\mathbf{x}, \mathbf{y})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y}) \tag{2.54}$$

# Chapter 3

## The time contour

### 3.1 The evolution operator

#### 3.1.1 Definition

Let  $|\Psi(t)\rangle$  be a solution to the TDSE then the time evolution operator  $\hat{U}(t, t')$  is defined by the relation

$$|\Psi(t)\rangle = \hat{U}(t, t')|\Psi(t')\rangle \quad (3.1)$$

i.e. it maps a wave function at time  $t'$  to a wave function at time  $t$ . It obviously satisfies the relation  $\hat{U}(t, t) = 1$ . If we differentiate Eq.(3.1) with respect to  $t$  and use the TDSE we obtain

$$i\partial_t \hat{U}(t, t')|\Psi(t')\rangle = \hat{H}(t)\hat{U}(t, t')|\Psi(t')\rangle \quad (3.2)$$

Since  $|\Psi(t')\rangle$  is arbitrary we find that

$$i\partial_t \hat{U}(t, t') = \hat{H}(t)\hat{U}(t, t') \quad (3.3)$$

On the other hand if we differentiate Eq.(3.1) with respect to  $t'$  we obtain

$$0 = (i\partial_{t'} \hat{U}(t, t')|\Psi(t')\rangle) + \hat{U}(t, t')\hat{H}(t')|\Psi(t')\rangle \quad (3.4)$$

This must be again true for any  $|\Psi(t')\rangle$  and therefore we have

$$i\partial_{t'} \hat{U}(t, t') = -\hat{U}(t, t')\hat{H}(t') \quad (3.5)$$

We thus see that the evolution operator satisfies the relations

$$i\partial_t \hat{U}(t, t') = \hat{H}(t)\hat{U}(t, t') \quad (3.6)$$

$$i\partial_{t'} \hat{U}(t, t') = -\hat{U}(t, t')\hat{H}(t') \quad (3.7)$$

$$\hat{U}(t, t) = 1 \quad (3.8)$$



These relations completely define the properties of the evolution operator. If we integrate Eq.(3.6) from  $t'$  to  $t$  where  $t > t'$  we have

$$\hat{U}(t, t') - \hat{U}(t', t') = \int_{t'}^t d\bar{t}_1 \partial_{\bar{t}_1} \hat{U}(\bar{t}_1, t') = -i \int_{t'}^t d\bar{t}_1 \hat{H}(\bar{t}_1) \hat{U}(\bar{t}_1, t') \quad (3.9)$$

and we obtain the expression

$$\hat{U}(t, t') = 1 - i \int_{t'}^t d\bar{t}_1 \hat{H}(\bar{t}_1) \hat{U}(\bar{t}_1, t') \quad (3.10)$$

This expression can be iterated to give

$$\begin{aligned} \hat{U}(t, t') &= 1 + \sum_{n=1}^{\infty} (-i)^n \int_{t'}^t d\bar{t}_1 \int_{t'}^{\bar{t}_1} d\bar{t}_2 \dots \int_{t'}^{\bar{t}_{n-1}} d\bar{t}_n \hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n) \\ &= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^t d\bar{t}_1 \int_{t'}^{\bar{t}_1} d\bar{t}_2 \dots \int_{t'}^{\bar{t}_{n-1}} d\bar{t}_n T[\hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n)] \end{aligned} \quad (3.11)$$

where we in the last step could make all integrals run from  $t'$  to  $t$  by introducing the time-ordered product

$$T[\hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n)] = \sum_P \theta(\bar{t}_{P(1)} - \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)} - \bar{t}_{P(n)}) \hat{H}(\bar{t}_{P(1)}) \dots \hat{H}(\bar{t}_{P(n)}) \quad (3.12)$$

where  $P$  runs over all permutations of the numbers  $1 \dots n$ . The latter expression is known as the time-ordered product which orders the operators at the latest times to the left. Similarly we can integrate Eq.(3.7) from  $t$  to  $t'$  when  $t' > t$ . This gives

$$\hat{U}(t, t') - \hat{U}(t, t) = \int_t^{t'} d\bar{t}_1 \partial_{\bar{t}_1} \hat{U}(t, \bar{t}_1) = i \int_t^{t'} d\bar{t}_1 \hat{U}(t, \bar{t}_1) \hat{H}(\bar{t}_1) \quad (3.13)$$

and therefore we have

$$\hat{U}(t, t') = 1 + i \int_t^{t'} d\bar{t}_1 \hat{U}(t, \bar{t}_1) \hat{H}(\bar{t}_1) \quad (3.14)$$

Iteration of this equation now gives

$$\begin{aligned} \hat{U}(t, t') &= 1 + \sum_{n=1}^{\infty} i^n \int_t^{t'} d\bar{t}_1 \int_t^{\bar{t}_1} d\bar{t}_2 \dots \int_t^{\bar{t}_{n-1}} d\bar{t}_n \hat{H}(\bar{t}_n) \dots \hat{H}(\bar{t}_1) \\ &= 1 + \sum_{n=1}^{\infty} \frac{i^n}{n!} \int_t^{t'} d\bar{t}_1 \int_t^{\bar{t}_1} d\bar{t}_2 \dots \int_t^{\bar{t}_{n-1}} d\bar{t}_n \tilde{T}[\hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n)] \end{aligned} \quad (3.15)$$

where now we defined anti-chronological time-ordering by

$$\tilde{T}[\hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n)] = \sum_P \theta(\bar{t}_{P(1)} - \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)} - \bar{t}_{P(n)}) \hat{H}(\bar{t}_{P(n)}) \dots \hat{H}(\bar{t}_{P(1)}) \quad (3.16)$$

i.e the latest times are ordered to the right. We can this formally write

$$\hat{U}(t, t') = T \exp(-i \int_{t'}^t d\tau \hat{H}(\tau)) \quad \text{when } t' < t \quad (3.17)$$

$$\hat{U}(t, t') = \tilde{T} \exp(i \int_t^{t'} d\tau \hat{H}(\tau)) \quad \text{when } t' > t \quad (3.18)$$

### 3.1.2 Evolution of ensembles

In the remainder of these lectures we will discuss the evolution of systems that are originally in thermodynamic equilibrium. In that case statistical mechanics tells us that the expectation values of operators are given as traces of appropriate ensembles. Let us therefore recall some basic definitions. The trace of an operator  $\hat{A}$  is defined as

$$\text{Tr} \{ \hat{A} \} = \sum_i \langle \Psi_i | \hat{A} | \Psi_i \rangle \quad (3.19)$$

where  $\{ |\Psi_i\rangle \}$  is a complete set in Fock space. The trace is independent of chosen set. This is easily seen by insertion of a complete set:

$$\begin{aligned} \sum_i \langle \Phi_i | \hat{A} | \Phi_i \rangle &= \sum_{i,j} \langle \Phi_i | \hat{A} | \Psi_j \rangle \langle \Psi_j | \Phi_i \rangle \\ &= \sum_{i,j} \langle \Psi_j | \Phi_i \rangle \langle \Phi_i | \hat{A} | \Psi_j \rangle = \sum_j \langle \Psi_j | \hat{A} | \Psi_j \rangle \end{aligned} \quad (3.20)$$

If we now consider a system at temperature  $T$  then its equilibrium expectation value of operator  $\hat{O}$  in the grand canonical ensemble is given by

$$\langle \hat{O} \rangle = \frac{\sum_i \langle \Psi_i | \hat{O} | \Psi_i \rangle e^{-\beta(E_i - \mu N_i)}}{\sum_i e^{-\beta(E_i - \mu N_i)}} \quad (3.21)$$

where  $\beta = 1/k_B T$  and  $k_B$  is the Boltzmann constant and where  $|\Psi_i\rangle$  present energy eigenstates of the system. This expression can equivalently be written as

$$\langle \hat{O} \rangle = \text{Tr} \{ \hat{\rho} \hat{O} \} \quad (3.22)$$

where we defined

$$\hat{\rho} = \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{\text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})}} \quad (3.23)$$

When we apply an external field to a system initially in thermodynamic equilibrium, it will subsequently evolve in time. It is this time-dependence that we want to study. Our Hamiltonian will have the general form.

$$\hat{H}(t) = \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) h(\mathbf{r}, t) \hat{\psi}(\mathbf{x}) + \frac{1}{2} \int \int d\mathbf{x}_1 d\mathbf{x}_2 \hat{\psi}^\dagger(\mathbf{x}_1) \hat{\psi}^\dagger(\mathbf{x}_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \hat{\psi}(\mathbf{x}_2) \hat{\psi}(\mathbf{x}_1), \quad (3.24)$$

where

$$h(\mathbf{r}, t) = \frac{1}{2} [-i\nabla + \mathbf{A}(\mathbf{r}, t)]^2 + v(\mathbf{r}, t) - \mu. \quad (3.25)$$

In the latter equation we introduced external potential  $v(\mathbf{r}, t)$  and vector potential  $\mathbf{A}(\mathbf{r}, t)$  which are switched on at  $t = t_0$ , i.e for  $t < t_0$  our Hamiltonian will be time-independent. Note that we also included the chemical potential in the definition of  $h$ . This means that we can simplify the expression of the statistical operator  $\hat{\rho}$  to

$$\hat{\rho} = \frac{e^{-\beta \hat{H}_0}}{\text{Tr} e^{-\beta \hat{H}_0}} \quad (3.26)$$

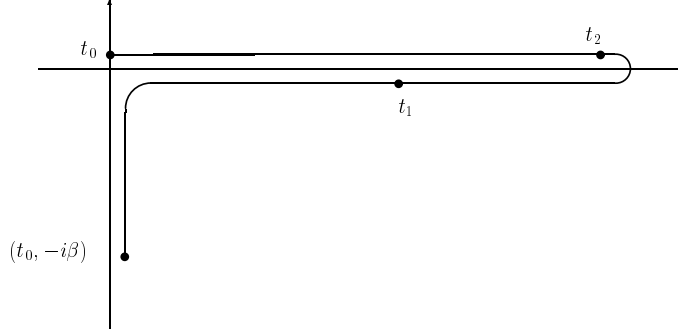


Figure 3.1: Keldysh contour. The forward and backward parts of the contour are on the real axis but are plotted slightly off this axis to display the two branches more clearly.

where we denote by  $\hat{H}_0$  the Hamiltonian for times  $t < t_0$ . After we switch on an external field the initial equilibrium ensemble will evolve in time and the new expectation value becomes

$$\langle \hat{O}(t) \rangle = \frac{\sum_i \langle \Psi_i(t) | \hat{O} | \Psi_i(t) \rangle e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = \text{Tr} \left\{ \hat{\rho} \hat{O}_H(t) \right\} \quad (3.27)$$

where

$$\hat{O}_H(t) = \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, t_0) \quad (3.28)$$

is the operator in the Heisenberg picture. Our task is now to evaluate such expectation values. First we will analyze the expression Eq.(3.27) a bit further.

## 3.2 Contour ordering

### 3.2.1 Definition of the contour

The operator  $e^{-\beta \hat{H}_0}$  can now be regarded as an evolution operator in imaginary time, i.e.

$$\hat{U}(t_0 - i\beta, t_0) = e^{-\beta \hat{H}_0} \quad (3.29)$$

if we define  $\hat{H}(t)$  to be equal to  $\hat{H}_0$  on the contour running straight from  $t_0$  to  $t_0 - i\beta$  in the complex time plane. We can therefore rewrite our expression for the expectation value as

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t) \hat{O} \hat{U}(t, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \quad (3.30)$$

If we read the time arguments of the evolution operators in the numerator of this expression from left to right we may say that the system evolves from  $t_0$  along the real time axis to  $t$  after which the operator  $\hat{O}$  acts. Then the system evolves back along the real axis from time  $t$  to  $t_0$  and finally parallel to the imaginary axis from  $t_0$  to  $t_0 - i\beta$ . A corresponding contour, originally introduced by Keldysh [1], is displayed in Fig. 3.1. With this observation we rewrite Eq.(3.30) as

$$\langle \hat{O}(t) \rangle = \frac{\text{Tr} \left\{ T_C [\exp(-i \int_C d\bar{t} \hat{H}(\bar{t})) \hat{O}(t)] \right\}}{\text{Tr} \left\{ T_C [\exp(-i \int_C d\bar{t} \hat{H}(\bar{t}))] \right\}} \quad (3.31)$$

where we define

$$T_C [\exp(-i \int_C d\bar{t} \hat{H}(\bar{t})) \hat{O}(t)] \equiv \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_C d\bar{t}_1 \dots d\bar{t}_n T_C [\hat{O}(t) \hat{H}(\bar{t}_1) \dots \hat{H}(\bar{t}_n)] \quad (3.32)$$

and we further defined the contour-ordered product

$$T_C [\hat{A}_1(\bar{t}_1) \dots \hat{A}_n(\bar{t}_n)] = \sum_P \theta(\bar{t}_{P(1)}, \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)}, \bar{t}_{P(n)}) \hat{A}_{P(1)}(\bar{t}_{P(1)}) \dots \hat{A}_{P(n)}(\bar{t}_{P(n)}) \quad (3.33)$$

where  $\theta(t_1, t_2)$  are contour step functions  $\theta$  generalized to arguments on the contour [2],

$$\theta(t_1, t_{1'}) = \begin{cases} 1 & \text{if } t_1 \text{ is later than } t_{1'} \text{ on the contour} \\ 0 & \text{otherwise} \end{cases} \quad (3.34)$$

For instance, time  $t_1$  in Fig. 3.1 is later than time  $t_2$  on the contour. All the time-integrals in Eq.(3.32) are taken along the contour.

### 3.2.2 Functional derivatives and the time-dependence of expectation values

This observation motivates us to define the following action functional

$$S = i \ln \text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}, \quad (3.35)$$

where we define the evolution operator on the contour as

$$\hat{U}(t, t') = T_C \exp(-i \int_{t'}^t d\bar{t} \hat{H}(\bar{t})). \quad (3.36)$$

Let us now see how this functional can be used as a generating functional by making variations with respect to parameters in the Hamiltonian. To do this one needs to consider changes in  $\hat{U}$ . When we make a perturbation  $\delta\hat{V}(t)$  in the Hamiltonian we have using Eqs.(3.6), (3.7) and (3.8) :

$$i\partial_t \delta\hat{U}(t, t') = \delta\hat{V}(t) \hat{U}(t, t') + \hat{H}(t) \delta U(t, t') \quad (3.37)$$

$$i\partial_{t'} \delta\hat{U}(t, t') = -\hat{U}(t, t') \delta\hat{V}(t') - \delta\hat{U}(t, t') \hat{H}(t') \quad (3.38)$$

$$\delta\hat{U}(t, t) = 0 \quad (3.39)$$

The solution to this equation is given by

$$\delta\hat{U}(t, t') = -i \int_{t'}^t d\tau \hat{U}(t, \tau) \delta\hat{V}(\tau) \hat{U}(\tau, t') \quad (3.40)$$

from which variations in the action can be calculated.

#### Exercise

Check that Eq.(3.40) is a solution to Eqs.(3.37) and Eq.(3.38) satisfying boundary condition

Eq.(3.39).

For instance, if we choose

$$\delta\hat{V}(t) = \int d\mathbf{x} \delta v(\mathbf{x}t) \hat{n}(\mathbf{x}) \quad (3.41)$$

where  $\hat{n}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$  is the density operator we have

$$\frac{\delta\hat{U}(t_0 - i\beta, t_0)}{\delta v(\mathbf{x}t)} = -i\hat{U}(t_0 - i\beta, t)\hat{n}(\mathbf{x})\hat{U}(t, t_0) = -i\hat{U}(t_0 - i\beta, t_0)\hat{n}_H(\mathbf{x}t) \quad (3.42)$$

From this equation we have

$$\frac{\delta S}{\delta v(\mathbf{x}t)} = \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t)\hat{n}(\mathbf{x})\hat{U}(t, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} = \langle \hat{n}(\mathbf{x}, t) \rangle \quad (3.43)$$

Similarly we can also calculate the change in expectation values.

$$\begin{aligned} \frac{\delta}{\delta v(\mathbf{x}_2 t_2)} \langle \hat{O}(t_1) \rangle &= \frac{\delta}{\delta v(\mathbf{x}_2 t_2)} \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_1)\hat{O}(t_1)\hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &= -i\theta(t_1, t_2) \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_1)\hat{O}(t_1)\hat{U}(t_1, t_2)\hat{n}(\mathbf{x}_2)\hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &\quad -i\theta(t_2, t_1) \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2)\hat{n}(\mathbf{x}_2)\hat{U}(t_2, t_1)\hat{O}(t_1)\hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &\quad +i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_1)\hat{O}(t_1)\hat{U}(t_1, t_0) \right\} \text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2)\hat{n}(\mathbf{x}_2)\hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\} \text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \end{aligned} \quad (3.44)$$

where the last term follows from differentiation of the denominator. The equation (3.44) can be rewritten as

$$\frac{\delta \langle \hat{O}(t_1) \rangle}{\delta v(\mathbf{x}_2 t_2)} = -i\theta(t_1, t_2) \langle \hat{O}_H(t_1)\hat{n}_H(\mathbf{x}_2 t_2) \rangle - i\theta(t_2, t_1) \langle \hat{n}_H(\mathbf{x}_2 t_2)\hat{O}_H(t_1) \rangle + i \langle \hat{O}(t_1) \rangle \langle \hat{n}_H(\mathbf{x}_2 t_2) \rangle \quad (3.45)$$

If we define the fluctuation operator

$$\Delta\hat{O}_H(\mathbf{x}t) = \hat{O}_H(\mathbf{x}t) - \langle \hat{O}_H(\mathbf{x}t) \rangle \quad (3.46)$$

this can be rewritten as

$$\begin{aligned} \frac{\delta \langle \hat{O}(t_1) \rangle}{\delta v(\mathbf{x}_2 t_2)} &= -i\theta(t_1, t_2) \langle \Delta\hat{O}_H(t_1)\Delta\hat{n}_H(\mathbf{x}_2 t_2) \rangle - i\theta(t_2, t_1) \langle \Delta\hat{n}_H(\mathbf{x}_2 t_2)\Delta\hat{O}_H(t_1) \rangle \\ &= -i \langle T_C[\Delta\hat{O}_H(t_1)\Delta\hat{n}_H(\mathbf{x}_2 t_2)] \rangle \end{aligned} \quad (3.47)$$

Similarly we can calculate derivatives of time-ordered products. We have

$$\begin{aligned} \frac{\delta \langle T_C[\hat{A}(t_1)\hat{B}(t_2)] \rangle}{\delta v(\mathbf{x}_3 t_3)} &= -i \langle T_C[\hat{A}(t_1)\hat{B}(t_2)\hat{n}_H(\mathbf{x}_3 t_3)] \rangle + i \langle \hat{n}_H(\mathbf{x}_3 t_3) \rangle \langle T_C[\hat{A}(t_1)\hat{B}(t_2)] \rangle \\ &= -i \langle T_C[\hat{A}(t_1)\hat{B}(t_2)\Delta\hat{n}_H(\mathbf{x}_3 t_3)] \rangle \end{aligned} \quad (3.48)$$

---

**Exercise**Prove relation (3.48)

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We finally consider the time-dependence of expectation values and consider the time-derivative of an expectation value  $\langle \hat{O}(t) \rangle$ . We then can calculate using Eqs.(3.6) and Eq.(3.7) :

$$\begin{aligned} i\partial_t \hat{O}_H(t) &= i\partial_t \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, t_0) = -\hat{U}(t_0, t) \hat{H}(t) \hat{O}(t) \hat{U}(t, t_0) \\ &\quad + \hat{U}(t_0, t) \hat{O}(t) \hat{H}(t) \hat{U}(t, t_0) + i\hat{U}(t_0, t) \partial_t \hat{O}(t) \hat{U}(t, t_0) \\ &= \hat{U}(t_0, t) \left\{ [\hat{O}(t), \hat{H}(t)] + i\partial_t \hat{O}(t) \right\} \hat{U}(t, t_0) \\ &= [\hat{O}_H(t), \hat{H}_H(t)] + i(\partial_t \hat{O}(t))_H \end{aligned} \quad (3.49)$$

where in the last step we used that for two operators  $\hat{A}$  and  $\hat{B}$  we have

$$\begin{aligned} \hat{U}(t_0, t) \hat{A}(t) \hat{B}(t) \hat{U}(t, t_0) &= \hat{U}(t_0, t) \hat{A}(t) \hat{U}(t, t_0) \hat{U}(t_0, t) \hat{B}(t) \hat{U}(t, t_0) \\ &= \hat{A}_H(t) \hat{B}_H(t) \end{aligned} \quad (3.50)$$

When we use expression (3.49) in the definition of the expectation value (3.30) we obtain

$$i\partial_t \langle \hat{O}(t) \rangle = \langle [\hat{O}_H(t), \hat{H}_H(t)] \rangle + i\langle (\partial_t \hat{O}(t))_H \rangle \quad (3.51)$$

### 3.2.3 Calculations with contour-ordered functions

In this section we will derive some relations that we will use later on. For simplicity we will introduce the notation  $i = \mathbf{x}_1 t_i$  for the space-time variables. In the previous section we saw that differentiation of expectation values naturally led to the consideration of contour-ordered operators of the form:

$$\langle T_C[\hat{A}(1)\hat{B}(2)] \rangle = \theta(t_1, t_2) \langle \hat{A}(1)\hat{B}(2) \rangle + \theta(t_2, t_1) \langle \hat{B}(2)\hat{A}(1) \rangle \quad (3.52)$$

We therefore consider general functions of the form

$$a(t, t') = a^\delta(t) \delta(t, t') + \theta(t, t') a^>(t, t') + \theta(t', t) a^<(t, t') \quad (3.53)$$

where the delta function on the contour is defined as  $\partial_t \theta(t, t')$ . A function of this form is said to belong to Keldysh space. When we consider the equation of motion of the Green function later we have to calculate contour integrals of products of such functions, i.e. function of the form

$$c(t, t') = \int_C d\bar{t} a(t, \bar{t}) b(\bar{t}, t') \quad (3.54)$$

where both  $a$  and  $b$  belong to Keldysh space. We will see that such a function also belongs to Keldysh space. Let us work out this integral. We have :

$$\begin{aligned} c(t, t') &= a(t, t') b^\delta(t') + a^\delta(t) b(t, t') \\ &+ \int_C d\bar{t} \left[ \theta(t, \bar{t}) \theta(\bar{t}, t') a^> b^> + \theta(t, \bar{t}) \theta(t', \bar{t}) a^> b^< + \theta(\bar{t}, t) \theta(\bar{t}, t') a^< b^> + \theta(\bar{t}, t) \theta(t', \bar{t}) a^> b^> \right] \end{aligned} \quad (3.55)$$

We can now consider several cases let  $t > t'$  on the contour and be real. Then we have

$$c^>(t, t') = a^>(t, t')b^\delta(t') + a^\delta(t)b^>(t, t') + \int_{t'}^t d\bar{t} a^>(t, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^{t'} d\bar{t} a^>(t, \bar{t})b^<(\bar{t}, t') + \int_t^{t_0-i\beta} d\bar{t} a^<(t, \bar{t})b^>(\bar{t}, t') \quad (3.56)$$

We denote

$$a^<(t, t_0 - i\tau) = a^\lceil(t, \tau) \quad (3.57)$$

$$a^>(t_0 - i\tau, t) = a^\lceil(\tau, t) \quad (3.58)$$

This notation is quite suggestive when one reads the symbols  $\lceil$  and  $\lrcorner$  from left to right. For instance  $\lrcorner$  has a horizontal segment followed by a vertical one; correspondingly  $a^\lceil$  has a first argument that is real (and thus lies on the horizontal axis) and a second argument that is imaginary (and lies on the vertical axis). With the notations of Eq.(3.57) and Eq.(3.58) we can rewrite expression (3.56) as

$$c^>(t, t') = a^>(t, t')b^\delta(t') + a^\delta(t)b^>(t, t') + \int_{t_0}^t d\bar{t} [a^>(t, \bar{t}) - a^<(t, \bar{t})]b^>(\bar{t}, t') - \int_{t_0}^{t'} d\bar{t} a^>(t, \bar{t})[b^>(\bar{t}, t') - b^<(\bar{t}, t')] - i \int_0^\beta d\tau a^\lceil(t, \tau)b^\lrcorner(\tau, t') \quad (3.59)$$

When we define the retarded and advanced functions in physical time as

$$a^R(t, t') = a^\delta(t)\delta(t - t') + \theta(t - t')[a^>(t, t') - a^<(t, t')] \quad (3.60)$$

$$a^A(t, t') = a^\delta(t)\delta(t - t') - \theta(t' - t)[a^>(t, t') - a^<(t, t')] \quad (3.61)$$

then Eq.(3.59) can be written shortly as

$$c^>(t, t') = \int_{t_0}^\infty d\bar{t} a^R(t, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^\infty d\bar{t} a^>(t, \bar{t})b^A(\bar{t}, t) - i \int_0^\beta d\tau a^\lceil(t, \tau)b^\lrcorner(\tau, t') \quad (3.62)$$

This expression can be even more simplified when we introduce the notation

$$a \cdot b = \int_{t_0}^\infty d\bar{t} a(\bar{t}) b(\bar{t}) \quad (3.63)$$

$$a \star b = -i \int_0^\beta d\tau a(\tau) b(\tau) \quad (3.64)$$

Then we simply find

$$c^> = a^R \cdot b^> + a^> \cdot b^A + a^\lceil \star b^\lrcorner \quad (3.65)$$

From Eq.(3.56) we can also derive an expression when  $t > t'$  on the contour and when  $t$  is on the imaginary part of the contour  $t = t_0 - i\tau$ . Equation (3.55) then becomes

$$c^\lrcorner(\tau, t') = c^>(t_0 - i\tau, t') = a^>(t_0 - i\tau, t')b^\delta(t') + a^\delta(t_0 - i\tau)b^>(t_0 - i\tau, t') + \int_{t'}^{t_0-i\tau} d\bar{t} a^>(t_0 - i\tau, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^{t'} d\bar{t} a^>(t_0 - i\tau, \bar{t})b^<(\bar{t}, t') + \int_{t_0-i\tau}^{t_0-i\beta} d\bar{t} a^<(t, \bar{t})b^>(\bar{t}, t') \quad (3.66)$$

This expression can be rewritten as

$$\begin{aligned}
c^\lceil(\tau, t') &= a^\lceil(\tau, t')b^\delta(t') + a^\delta(t_0 - i\tau)b^\lceil(\tau, t') - \int_{t_0}^{t'} d\bar{t} a^\lceil(\tau, \bar{t})[b^\rceil(\bar{t}, t') - b^\lessdot(\bar{t}, t')] \\
&+ \int_{t_0}^{t_0 - i\tau} d\bar{t} a^\gtrless(t_0 - i\tau, \bar{t})b^\lceil(\bar{t}, t') + \int_{t_0 - i\tau}^{t_0 - i\beta} d\bar{t} a^\lessdot(t_0 - i\tau, \bar{t})b^\lceil(\bar{t}, t') \\
&= \int_{t_0}^{\infty} d\bar{t} a^\lceil(\tau, \bar{t})b^A(\bar{t}, t') - i \int_0^\beta d\bar{\tau} a^M(\tau, \bar{\tau})b^\lceil(\bar{\tau}, t')
\end{aligned} \tag{3.67}$$

where, for convenience, we defined the Matsubara function  $a^M$  as the function  $a$  restricted to the imaginary part of the contour

$$a^M(\tau_1, \tau_2) = i a^\delta(\bar{t}_1)\delta(\tau_1 - \tau_2) + \theta(\tau_1 - \tau_2)a^\gtrless(\bar{t}_1, \bar{t}_2) + \theta(\tau_2 - \tau_1)a^\lessdot(\bar{t}_2, \bar{t}_1) \tag{3.68}$$

where in this expression  $\bar{t}_1 = t_0 - i\tau_1$  and  $\bar{t}_2 = t_0 - i\tau_2$ . Equation (3.67) can in condensed notation be rewritten as

$$c^\lceil = a^\lceil \cdot b^A + a^M \star b^\lceil \tag{3.69}$$

Finally, if we let  $t$  and  $t'$  be both on the imaginary part of the contour then one readily sees that the real part of the contour does not contribute in Eq.(3.54) and we immediately find that

$$c^M = a^M \star b^M \tag{3.70}$$

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**Exercise**

Derive the relations

$$c^\lessdot = a^R \cdot b^\lessdot + a^\lessdot \cdot b^A + a^\lceil \star b^\lceil \tag{3.71}$$

$$c^\lceil = a^R \cdot b^\lceil + a^\lceil \star b^M \tag{3.72}$$


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## Chapter 4

# The Green function

### 4.1 Definition

Before we give the definition of the Green function we first extend our definition of time-ordering slightly. So far we only considered operators at a particular time that consist of products of an even number of field operators, such as the Hamiltonian and operators that represent observables. Such operators we call non-fermionic (they are, however, not bosonic in general since they need not satisfy bosonic commutation relations). However, in the following we will also consider time-ordering of fermionic field operators themselves. To treat this case the definition of time-ordering is extended to

$$T_C[\hat{A}_1(\bar{t}_1) \dots \hat{A}_n(\bar{t}_n)] = \sum_P (-1)^{F_P} \theta(\bar{t}_{P(1)}, \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)}, \bar{t}_{P(n)}) \hat{A}_{P(1)}(\bar{t}_{P(1)}) \dots \hat{A}_{P(n)}(\bar{t}_{P(n)}) \quad (4.1)$$

where  $F_P$  is the number of times that a fermionic operator gets interchanged with another fermionic operator in the permutation  $P$ . Let us give an example. Let  $\hat{O}$  be a non-fermionic operator that consist of products of an even number of field operators. Then according to our definition we have

$$\begin{aligned} T_C[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{O}(3)] &= \\ &\theta(t_1, t_2) \theta(t_2, t_3) \hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{O}(3) + \theta(t_1, t_3) \theta(t_3, t_2) \hat{\psi}_H(1)\hat{O}(3)\hat{\psi}_H^\dagger(2) \\ &+ \theta(t_3, t_1) \theta(t_1, t_2) \hat{O}(3)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) - \theta(t_2, t_1) \theta(t_1, t_3) \hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\hat{O}(3) \\ &- \theta(t_2, t_3) \theta(t_3, t_1) \hat{\psi}_H^\dagger(2)\hat{O}(3)\hat{\psi}_H(1) - \theta(t_3, t_2) \theta(t_2, t_1) \hat{O}(3)\hat{\psi}_H^\dagger(2)\hat{\psi}_H(1) \end{aligned} \quad (4.2)$$

We see that the last three terms gained a minus sign as  $\hat{\psi}_H^\dagger(2)$  and  $\hat{\psi}_H(1)$  were interchanged in these terms. With this definition of time-ordering we now define the one-particle Green's function  $G$  as

$$\begin{aligned} G(1, 2) &= \frac{1}{i} \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) T_C \left[ \hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) \right] \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &= -i \langle T_C[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)] \rangle, \end{aligned} \quad (4.3)$$

This can be written in the form

$$G(1, 2) = \theta(t_1, t_2)G^>(1, 2) + \theta(t_2, t_1)G^<(1, 2). \quad (4.4)$$

where we introduced the greater and lesser Green functions  $G^>$  and  $G^<$  according to

$$G^>(1, 2) = -i\langle\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\rangle \quad (4.5)$$

$$G^<(1, 2) = i\langle\hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\rangle \quad (4.6)$$

Let us now derive the boundary conditions that  $G$  satisfies. If we consider the Green function at  $t_1 = t_0 - i\beta$  and use the cyclic property of the trace we find

$$\begin{aligned} G(\mathbf{x}_1 t_0 - i\beta, 2) &= \frac{1}{i} \frac{\text{Tr} \left\{ \hat{\psi}(\mathbf{x}_1) \hat{U}(t_0 - i\beta, t_2) \hat{\psi}^\dagger(\mathbf{x}_2) \hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &= \frac{1}{i} \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2) \hat{\psi}^\dagger(\mathbf{x}_2) \hat{U}(t_2, t_0) \hat{\psi}(\mathbf{x}_1) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} = -G(\mathbf{x}_1 t_0, 2). \end{aligned} \quad (4.7)$$

The Green function defined in Eq. (4.3) therefore obeys the boundary condition  $G(\mathbf{x}_1 t_0, 2) = -G(\mathbf{x}_1 t_0 - i\beta, 2)$ . The property  $G(1, \mathbf{x}_2 t_0) = -G(1, \mathbf{x}_2 t_0 - i\beta)$  for the other argument is likewise easily verified. These boundary conditions are sometimes referred to as the Kubo-Martin-Schwinger conditions [3, 4, 5]. Similar boundary conditions are satisfied by the usual equilibrium temperature Green function which, in fact, is obtained for the special case where the time arguments are located on the contour along the imaginary axis  $t_0$  to  $t_0 - i\beta$ , where the Hamiltonian is time-independent. Analogously to the one-particle Green function one can further define the  $n$ -particle Green function

$$G_n(1, \dots, n, 1', \dots, n') = (-i)^n \langle T_C [\hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \rangle \quad (4.8)$$

Also these Green function satisfy Kubo-Martin-Schwinger boundary conditions. One can derive a set of so-called hierarchy equations of motion that relate the  $n$ -particle Green function to the  $n \pm 1$ -particle Green functions.

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### Exercise

Derive the condition

$$G(1, \mathbf{x}_2 t_0) = -G(1, \mathbf{x}_2 t_0 - i\beta) \quad (4.9)$$


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## 4.2 Physical content

### 4.2.1 Expectation values

The Green function  $G$  is a basic ingredient in a diagrammatic perturbation expansion and it directly gives us the expectation values of one-particle operators. A one-body operator  $\hat{O}$  can be expressed

as

$$\langle \hat{O}(t) \rangle = \int d\mathbf{x} o(\mathbf{x}'t) \langle \hat{\psi}^\dagger(\mathbf{x}, t) \hat{\psi}(\mathbf{x}'t) \rangle \Big|_{\mathbf{x}'=\mathbf{x}} = -i \int d\mathbf{x} o(\mathbf{x}'t) G^<(\mathbf{x}t, \mathbf{x}'t) \Big|_{\mathbf{x}'=\mathbf{x}} \quad (4.10)$$

For instance, if we denote by  $1^+$  the limit to  $t_1$  from above on the contour, the density is quite simply

$$\langle \hat{n}(1) \rangle = -iG(1, 1^+) \quad (4.11)$$

and the current density is

$$\langle \mathbf{j}(1) \rangle = -i \left\{ \left[ \frac{\nabla_1}{2i} - \frac{\nabla_{1'}}{2i} + \mathbf{A}(1) \right] G(1, 1') \right\}_{1'=1^+} \quad (4.12)$$

The calculated observables will obviously depend on what approximation scheme we use to obtain  $G$ . It is therefore important that these approximations are such that the calculated observables satisfy the macroscopic conservation laws, like e.g. the continuity equation,  $\partial_t \langle \hat{n} \rangle = -\nabla \cdot \langle \mathbf{j} \rangle$ . Such approximations are called *conserving approximations* and will be discussed later on.

## 4.2.2 Removal and addition energies

We will now derive a useful relation for the Green function that clearly displays its physical content. This relation is known as the Lehmann representation. We first consider the Green function on the imaginary part of the contour. In that case we have  $t = -i\tau$  where  $\tau$  runs from 0 to  $\beta$  (we put the time  $t_0$  to zero without loss of generality). In that case we have

$$\begin{aligned} G(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) &= G^M(\mathbf{x}_1\tau_1, \mathbf{x}_2\tau_2) \\ &= \theta(\tau_1 - \tau_2)G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) + \theta(\tau_2 - \tau_1)G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) \end{aligned} \quad (4.13)$$

Let us first analyze  $G^<$ . We have

$$\begin{aligned} G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) &= i \langle \hat{\psi}^\dagger(\mathbf{x}_2, -i\tau_2) \hat{\psi}(\mathbf{x}_1, -i\tau_1) \rangle \\ &= i \frac{1}{Z} \sum_i \langle \Psi_i | e^{-\beta \hat{H}_0} e^{\hat{H}_0 \tau_2} \hat{\psi}^\dagger(\mathbf{x}_2) e^{-\hat{H}_0 \tau_2} e^{\hat{H}_0 \tau_1} \hat{\psi}(\mathbf{x}_1) e^{-\hat{H}_0 \tau_1} | \Psi_i \rangle \\ &= i \frac{1}{Z} \sum_{i,j} e^{-\beta E_i} e^{E_i(\tau_2 - \tau_1)} \langle \Psi_i | \hat{\psi}^\dagger(\mathbf{x}_2) e^{-\hat{H}_0 \tau_2} | \Psi_j \rangle \langle \Psi_j | e^{\hat{H}_0 \tau_1} \hat{\psi}(\mathbf{x}_1) | \Psi_i \rangle \\ &= i \frac{1}{Z} \sum_{i,j} e^{-\beta E_i} e^{(E_i - E_j)(\tau_2 - \tau_1)} \langle \Psi_i | \hat{\psi}^\dagger(\mathbf{x}_2) | \Psi_j \rangle \langle \Psi_j | \hat{\psi}(\mathbf{x}_1) | \Psi_i \rangle \end{aligned} \quad (4.14)$$

where we defined  $Z = \text{Tr} \{ \hat{U}(t_0 - i\beta, t_0) \}$ . We can do a similar calculation for  $G^>$

$$\begin{aligned} G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) &= -i \langle \hat{\psi}(\mathbf{x}_1, -i\tau_1) \hat{\psi}^\dagger(\mathbf{x}_2, -i\tau_2) \rangle \\ &= -i \frac{1}{Z} \sum_i \langle \Psi_i | e^{-\beta \hat{H}_0} e^{\hat{H}_0 \tau_1} \hat{\psi}(\mathbf{x}_1) e^{-\hat{H}_0 \tau_1} e^{\hat{H}_0 \tau_2} \hat{\psi}^\dagger(\mathbf{x}_2) e^{-\hat{H}_0 \tau_2} | \Psi_i \rangle \\ &= -i \frac{1}{Z} \sum_{i,j} e^{-\beta E_i} e^{E_i(\tau_1 - \tau_2)} \langle \Psi_i | \hat{\psi}(\mathbf{x}_1) e^{-\hat{H}_0 \tau_1} | \Psi_j \rangle \langle \Psi_j | e^{\hat{H}_0 \tau_2} \hat{\psi}^\dagger(\mathbf{x}_2) | \Psi_i \rangle \\ &= -i \frac{1}{Z} \sum_{i,j} e^{-\beta E_i} e^{(E_i - E_j)(\tau_1 - \tau_2)} \langle \Psi_i | \hat{\psi}(\mathbf{x}_1) | \Psi_j \rangle \langle \Psi_j | \hat{\psi}^\dagger(\mathbf{x}_2) | \Psi_i \rangle \end{aligned} \quad (4.15)$$

Let us check the anti-periodicity conditions. We have for  $0 \leq \tau_2 \leq \beta$  :

$$G(\mathbf{x}_1, 0, \mathbf{x}_2, -i\tau_2) = G^<(\mathbf{x}_1, 0, \mathbf{x}_2, -i\tau_2) \quad (4.16)$$

$$G(\mathbf{x}_1, -i\beta, \mathbf{x}_2, -i\tau_2) = G^>(\mathbf{x}_1, -i\beta, \mathbf{x}_2, -i\tau_2) \quad (4.17)$$

and therefore we must have

$$G^<(\mathbf{x}_1, 0, \mathbf{x}_2, -i\tau_2) = -G^>(\mathbf{x}_1, -i\beta, \mathbf{x}_2, -i\tau_2) \quad (4.18)$$

From the explicit expressions Eq.(4.15) and Eq.(4.14) we see that this relation is indeed satisfied. When we consider finite electronic systems we can often take the zero temperature limit ( $\beta \rightarrow \infty$ ). In that case we can choose the chemical potential such that  $E_0 < 0$  and  $E_i > 0$ . If the ground state then has  $N$  particles we find for  $G^{\lessgtr}$  the following expressions

$$G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = i \sum_j e^{(E_{N,0} - E_{N-1,j})(\tau_2 - \tau_1)} \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{x}_2) | N-1, j \rangle \langle N-1, j | \hat{\psi}(\mathbf{x}_1) | \Psi_0 \rangle$$

$$G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = -i \sum_j e^{(E_{N,0} - E_{N+1,j})(\tau_1 - \tau_2)} \langle \Psi_0 | \hat{\psi}(\mathbf{x}_1) | N+1, j \rangle \langle N+1, j | \hat{\psi}^\dagger(\mathbf{x}_2) | \Psi_0 \rangle$$

where  $|N \pm 1, j\rangle$  denote  $N \pm 1$ -particle eigenstates of the system. The calculation above could, of course, also easily have been carried out in real time on the real axis provided we do not switch-on any time-dependent external fields. In that case we have (for simplicity in the zero-temperature limit)

$$G^<(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) = i \sum_j e^{i(E_{N,0} - E_{N-1,j})(t_2 - t_1)} \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{x}_2) | N-1, j \rangle \langle N-1, j | \hat{\psi}(\mathbf{x}_1) | \Psi_0 \rangle$$

$$G^>(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) = -i \sum_j e^{i(E_{N,0} - E_{N+1,j})(t_1 - t_2)} \langle \Psi_0 | \hat{\psi}(\mathbf{x}_1) | N+1, j \rangle \langle N+1, j | \hat{\psi}^\dagger(\mathbf{x}_2) | \Psi_0 \rangle$$

With the definitions of the so-called Feynman-Dyson amplitudes

$$g_j(\mathbf{x}_1) = \langle N-1, j | \hat{\psi}(\mathbf{x}_1) | \Psi_0 \rangle \quad (4.19)$$

$$f_j(\mathbf{x}_1) = \langle \Psi_0 | \hat{\psi}(\mathbf{x}_1) | N+1, j \rangle \quad (4.20)$$

These expressions simplify to

$$G^<(\mathbf{x}_1, \mathbf{x}_2; t_1 - t_2) = i \sum_j e^{i(E_{N,0} - E_{N-1,j})(t_2 - t_1)} g_j(\mathbf{x}_1) g_j^*(\mathbf{x}_2) \quad (4.21)$$

$$G^>(\mathbf{x}_1, \mathbf{x}_2; t_1 - t_2) = -i \sum_j e^{i(E_{N,0} - E_{N+1,j})(t_1 - t_2)} f_j(\mathbf{x}_1) f_j^*(\mathbf{x}_2) \quad (4.22)$$

We can now for the equilibrium situation define the spectral functions

$$A^{\lessgtr}(\mathbf{x}_1, \mathbf{x}_2; \omega) = i \int d\tau G^{\lessgtr}(\mathbf{x}_1, \mathbf{x}_2; \tau) e^{i\omega\tau} \quad (4.23)$$

We find the explicit expressions

$$A^<(\mathbf{x}_1, \mathbf{x}_2; \omega) = - \sum_j g_j(\mathbf{x}_1) g_j^*(\mathbf{x}_2) \delta(\omega - (E_{N,0} - E_{N-1,j})) \quad (4.24)$$

$$A^>(\mathbf{x}_1, \mathbf{x}_2; \omega) = \sum_j f_j(\mathbf{x}_1) f_j^*(\mathbf{x}_2) \delta(\omega + (E_{N,0} - E_{N+1,j})) \quad (4.25)$$

We thus see that Fourier transforming  $G^<$  gives a function that is peaked at the ionization energies of the system, whereas Fourier transforming  $G^>$  gives a function that is peaked at the addition energies or affinities. For instance, photo-electron spectra can directly be calculated from knowledge of  $A^<$ .

### 4.2.3 Excitation energies

The time-propagation of the Green function gives also the expectation values of the time-dependent one-body observables. A subsequent Fourier transformation then gives us also directly the excitation energies of the system. Let us illustrate this with the density operator. The time-dependent density is directly obtained from the Green function from Eq.(4.11). If we expand the density in powers of the external field we obtain

$$\begin{aligned}
\langle \hat{n}_H(1) \rangle &= n_0(\mathbf{x}_1) + \int d2 \frac{\delta \langle \hat{n}_H(1) \rangle}{\delta v(2)} v(2) + \frac{1}{2} \int d2d3 \frac{\delta^2 \langle \hat{n}_H(1) \rangle}{\delta v(2) \delta v(3)} v(2)v(3) + \dots \\
&= n_0(\mathbf{x}_1) + (-i) \int d2 \langle T_C [\Delta \hat{n}_H(1) \Delta \hat{n}_H(2)] \rangle v(2) \\
&\quad + \frac{(-i)^2}{2} \int d2d3 \langle T_C [\Delta \hat{n}_H(1) \Delta \hat{n}_H(2) \Delta \hat{n}_H(3)] \rangle v(2)v(3) + \dots
\end{aligned} \tag{4.26}$$

where we used Eqs.(3.47) and Eq.(3.48). If we undo the contour integrations we obtain the linear and higher order density response functions. Let us for instance consider the linear term. We write

$$\chi(1, 2) = -i \langle T_C [\Delta \hat{n}_H(1) \Delta \hat{n}_H(2)] \rangle = \theta(t_1, t_2) \chi^>(1, 2) + \theta(t_2, t_1) \chi^<(1, 2) \tag{4.27}$$

where

$$\chi^>(1, 2) = -i \langle \Delta \hat{n}_H(1) \Delta \hat{n}_H(2) \rangle \tag{4.28}$$

$$\chi^<(1, 2) = -i \langle \Delta \hat{n}_H(2) \Delta \hat{n}_H(1) \rangle \tag{4.29}$$

Then we have

$$\begin{aligned}
\langle \hat{n}_H(1) \rangle - n_0(\mathbf{x}_1) &= \int d2 \chi(1, 2) v(2) = \int_{t_0}^{t_1} d2 \chi^>(1, 2) v(2) + \int_{t_1}^{t_0} d2 \chi^<(1, 2) v(2) \\
&= \int_{t_0}^{t_1} d2 (\chi^>(1, 2) - \chi^<(1, 2)) v(2) = \int_{t_0}^{\infty} \chi_R(1, 2) v(2)
\end{aligned} \tag{4.30}$$

where we used that external perturbing field is zero on the imaginary part of the contour and we define the retarded response function as

$$\chi_R(1, 2) = \theta(t_1 - t_2) (\chi^>(1, 2) - \chi^<(1, 2)) = -i \theta(t_1 - t_2) \langle [\hat{n}_H(1), \hat{n}_H(2)] \rangle \tag{4.31}$$

and where we used that the commutators of two operators is the same as the commutators of the corresponding fluctuation operators. Now the operators  $\chi^{\lessgtr}$  have a similar Lehmann representation as the Green function. For instance in the zero temperature limit we have

$$\chi^<(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) = -i \sum_j e^{i(E_{N,0} - E_{N,j})(t_2 - t_1)} \langle \Psi_0 | \hat{n}(\mathbf{x}_2) | N, j \rangle \langle N, j | \hat{n}(\mathbf{x}_1) | \Psi_0 \rangle \tag{4.32}$$

This expression is very similar to that of  $G^<$ . The main difference is that instead of removal energies this expression contains particle-number conserving excitations. Fourier transformation of this quantity gives us the excitation spectrum of the system. Similar Lehmann representations exist for the higher order response functions that will play a role when we propagate the Green function in stronger external fields.

## Chapter 5

# The equations of motion

### 5.1 The self-energy

We now study the equation of motion for the Green function. Using the definition of operators in the Heisenberg picture, and the Hamiltonian as given in Eq. (3.24), the equation of motion for the field operators is

$$\begin{aligned} i\partial_{t_1}\hat{\psi}_H(1) &= [\hat{\psi}_H(1), \hat{H}_H(t_1)] \\ &= h(1)\hat{\psi}_H(1) + \int d2 w(1, 2)\hat{\psi}_H^\dagger(2)\hat{\psi}_H(2)\hat{\psi}_H(1) \end{aligned} \quad (5.1)$$

$$\begin{aligned} i\partial_{t_1}\hat{\psi}_H^\dagger(1) &= [\hat{\psi}_H^\dagger(1), \hat{H}_H(t_1)] \\ &= -h(1)\hat{\psi}_H^\dagger(1) - \int d2 w(1, 2)\hat{\psi}_H^\dagger(1)\hat{\psi}_H^\dagger(2)\hat{\psi}_H(2) \end{aligned} \quad (5.2)$$

where  $w(1, 2) = \delta(t_1, t_2)/|\mathbf{r}_1 - \mathbf{r}_2|$  is the Coulomb interaction. The notation  $\delta(t_1, t_2)$  again indicates that the time-arguments are on the contour. In deriving these expressions we used Eqs.(2.53) and (2.54) together with Eq.(3.49). Let us now take the time derivative of the Green function:

$$\begin{aligned} i\partial_{t_1}G(1, 2) &= i\partial_{t_1}\theta(t_1, t_2)G^>(1, 2) + i\partial_{t_1}\theta(t_2, t_1)G^<(1, 2) \\ &\quad + \theta(t_1, t_2)i\partial_{t_1}G^>(1, 2) + \theta(t_2, t_1)i\partial_{t_1}G^<(1, 2) \\ &= i\delta(t_1, t_2)[G^>(1, 2) - G^<(1, 2)] \\ &\quad - i\theta(t_1, t_2)\langle i\partial_{t_1}\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) \rangle + i\theta(t_2, t_1)\langle \hat{\psi}_H^\dagger(2)i\partial_{t_1}\hat{\psi}_H(1) \rangle \end{aligned} \quad (5.3)$$

For the first term in this expression we can use the anti-commutation relations at equal times

$$i\delta(t_1, t_2)[G^>(1, 2) - G^<(1, 2)] = \delta(t_1, t_2)\langle \{\hat{\psi}_H(\mathbf{x}_1, t_1), \hat{\psi}_H^\dagger(\mathbf{x}_2, t_1)\} \rangle = \delta(1, 2) \quad (5.4)$$

where  $\delta(1, 2) = \delta(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1, t_2)$ . Using Eqs.(5.1) in the last two terms of Eq.(5.3) we then obtain

$$\begin{aligned} i\partial_{t_1}G(1, 2) &= \delta(1, 2) + h(1)G(1, 2) \\ &\quad - i \int d3 w(1, 3) \left[ \theta(t_1, t_2)\langle \hat{\psi}_H^\dagger(3)\hat{\psi}_H(3)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) \rangle - \theta(t_2, t_1)\langle \hat{\psi}_H^\dagger(2)\hat{\psi}_H^\dagger(3)\hat{\psi}_H(3)\hat{\psi}_H(1) \rangle \right] \end{aligned} \quad (5.5)$$

Now in the last line of this equation the pair of operators  $\hat{\psi}_H^\dagger(3)\hat{\psi}_H(3) = \hat{n}_H(3)$  is actually evaluated at  $t_3 = t_1$  due to the presence of an equal-time delta function in  $w(1,3)$ . However, this pair of operators is always situated to the left of  $\hat{\psi}_H(1)$  and this ordering can thus also be obtained from

$$\begin{aligned} & \lim_{\delta \rightarrow 0} \langle T_C [\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)] \rangle \Big|_{t_3=t_1+\delta} \\ &= \theta(t_1, t_2) \langle \hat{n}_H(3)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) \rangle - \theta(t_2, t_1) \langle \hat{\psi}_H^\dagger(2)\hat{n}_H(3)\hat{\psi}_H(1) \rangle \Big|_{t_3=t_1} \end{aligned} \quad (5.6)$$

where  $t_1 + \delta$  means that the limit is taken from above on the contour. This equation also follows directly from Eq.(4.2) by taking  $\hat{O}(3) = \hat{n}_H(3)$ . If we then replace  $w(1,3)$  by  $w(1^+,3)$  where  $1^+ = \mathbf{x}_1, t_1 + \delta$  we can write Eq.(5.5) as

$$(i\partial_{t_1} - h(1))G(1,2) = \delta(1,2) - i \int d3 w(1^+,3) \langle T_C [\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)] \rangle \quad (5.7)$$

Using the definition of the two-particle Green function (4.8) we can also write

$$\langle T_C [\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)] \rangle = G_2(1,3,3^+,2) \quad (5.8)$$

We can therefore write the equation of motion as

$$[i\partial_{t_1} - h(1)]G(1,2) = \delta(1,2) - i \int d3 w(1^+,3)G_2(1,3,3^+,2). \quad (5.9)$$

Similarly one has the adjoint equation

$$[-i\partial_{t_2} - h(2)]G(1,2) = \delta(1,2) - i \int d3 w(2^+,3)G_2(1,3,3^+,2). \quad (5.10)$$

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### Exercise

Derive Eq.(5.10)

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The problem is that the equation of motion for  $G$  depends on the two-particle Green function  $G_2$ . Instead of propagating the equation with some approximate form of  $G_2$ , we introduce the electronic self energy  $\Sigma$ , such that the term  $-iG_2w$  is replaced with  $\Sigma G$ . We define the self-energy  $\Sigma$  and its adjoint  $\hat{\Sigma}$  by the equations

$$\int d2 \Sigma(1,2)G(2,1') = -i \int d2 w(1,2)G_2(1,2,2^+,1') \quad (5.11)$$

$$\int d2 G(1,2)\hat{\Sigma}(2,1') = -i \int d2 w(1',2)G_2(1,2,2^+,1') \quad (5.12)$$

It is not difficult to derive that  $\Sigma = \hat{\Sigma}$  for initial equilibrium conditions. To do this we first write Eqs.(5.1) and (5.2) in the following form:

$$(i\partial_{t_1} - h(1))\hat{\psi}_H(1) = \hat{i}_H(1) \quad (5.13)$$

$$(-i\partial_{t_1} - h(1))\hat{\psi}_H^\dagger(1) = \hat{i}_H^\dagger(1) \quad (5.14)$$

where we defined the operators

$$\hat{i}_H(1) = \int d2 w(1,2)\hat{\psi}_H^\dagger(2)\hat{\psi}_H(2)\hat{\psi}_H(1) \quad (5.15)$$

$$\hat{i}_H^\dagger(1) = \int d2 w(1,2)\hat{\psi}_H^\dagger(1)\hat{\psi}_H^\dagger(2)\hat{\psi}_H(2) \quad (5.16)$$

These operators are readily seen to be each others adjoints. In terms of these operators the equations of motion of the Green function become

$$(i\partial_{t_1} - h(1))G(1, 2) = \delta(1, 2) - i\langle T_C[\hat{i}_H(1)\hat{\psi}_H^\dagger(2)] \rangle \quad (5.17)$$

$$(-i\partial_{t_2} - h(2))G(1, 2) = \delta(1, 2) - i\langle T_C[\hat{\psi}_H(1)\hat{i}_H^\dagger(2)] \rangle \quad (5.18)$$

where from the derivation it is clear that the operators  $\hat{i}_H$  and  $\hat{i}_H^\dagger$  must be regarded as fermionic in the time-ordered product. From these equations we see immediately that

$$\int d3 \Sigma(1, 3)G(3, 2) = -i\langle T_C[\hat{i}_H(1)\hat{\psi}_H^\dagger(2)] \rangle \quad (5.19)$$

$$\int d3 G(1, 3)\hat{\Sigma}(3, 2) = -i\langle T_C[\hat{\psi}_H(1)\hat{i}_H^\dagger(2)] \rangle \quad (5.20)$$

From the equation of motion of the Green function we see that for the left hand sides of Eqs.(5.19) and (5.20) we can write

$$(-i\partial_{t_2} - h(2)) \int d3 \Sigma(1, 3)G(3, 2) = \Sigma(1, 2) + \int d3 d4 \Sigma(1, 3)G(3, 4)\hat{\Sigma}(4, 2) \quad (5.21)$$

$$(i\partial_{t_1} - h(1)) \int d3 G(1, 3)\hat{\Sigma}(3, 2) = \hat{\Sigma}(1, 2) + \int d3 d4 \Sigma(1, 3)G(3, 4)\hat{\Sigma}(4, 2) \quad (5.22)$$

whereas for the right hand sides we obtain

$$\begin{aligned} & -i(-i\partial_{t_2} - h(2))\langle T_C[\hat{i}_H(1)\hat{\psi}_H^\dagger(2)] \rangle \\ & = -\partial_{t_2}\theta(t_1, t_2)\langle \hat{i}_H(1)\hat{\psi}_H^\dagger(2) \rangle + \partial_{t_2}\theta(t_2, t_1)\langle \hat{\psi}_H^\dagger(2)\hat{i}_H(1) \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \\ & = \delta(t_1, t_2)\langle \{ \hat{i}_H(1), \hat{\psi}_H^\dagger(2) \} \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \end{aligned} \quad (5.23)$$

and

$$\begin{aligned} & -i(i\partial_{t_1} - h(1))\langle T_C[\hat{\psi}_H(1)\hat{i}_H^\dagger(2)] \rangle \\ & = \partial_{t_1}\theta(t_1, t_2)\langle \hat{\psi}_H(1)\hat{i}_H^\dagger(2) \rangle - \partial_{t_1}\theta(t_2, t_1)\langle \hat{i}_H^\dagger(2)\hat{\psi}_H(1) \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \\ & = \delta(t_1, t_2)\langle \{ \hat{\psi}_H(1), \hat{i}_H^\dagger(2) \} \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \end{aligned} \quad (5.24)$$

We have therefore obtained the relations

$$\begin{aligned} \Sigma(1, 2) & + \int d3 d4 \Sigma(1, 3)G(3, 4)\hat{\Sigma}(4, 2) \\ & = \delta(t_1, t_2)\langle \{ \hat{i}_H(1), \hat{\psi}_H^\dagger(2) \} \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \end{aligned} \quad (5.25)$$

$$\begin{aligned} \hat{\Sigma}(1, 2) & + \int d3 d4 \Sigma(1, 3)G(3, 4)\hat{\Sigma}(4, 2) \\ & = \delta(t_1, t_2)\langle \{ \hat{\psi}_H(1), \hat{i}_H^\dagger(2) \} \rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(2)] \rangle \end{aligned} \quad (5.26)$$

Now it is readily seen by computation that for the equal time parts on the left hand sides of Eqs.(5.25) and (5.26) we have

$$\langle \{ \hat{i}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) \} \rangle = \langle \{ \hat{\psi}_H(\mathbf{x}_1 t_1), \hat{i}_H^\dagger(\mathbf{x}_2 t_1) \} \rangle \quad (5.27)$$



and therefore Eqs.(5.25) and (5.26) immediately imply that

$$\Sigma(1, 2) = \hat{\Sigma}(1, 2) \quad (5.28)$$

We further see from Eq.(5.25) that  $\Sigma$  has the following structure

$$\Sigma(1, 2) = \Sigma^\delta(1, 2) + \theta(t_1, t_2)\Sigma^>(1, 2) + \theta(t_2, t_1)\Sigma^<(1, 2) \quad (5.29)$$

where the equal-time singular part of  $\Sigma$  is given by

$$\Sigma^\delta(1, 2) = \delta(t_1, t_2)\langle\{\hat{i}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1)\}\rangle \quad (5.30)$$

This term is really worked out in more explicit form using the equal time anti-commutation relations of the field operators

$$\begin{aligned} & \{\hat{i}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1)\} \\ &= \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \left( \hat{\psi}_H^\dagger(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_1 t_1) \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) + \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) \hat{\psi}_H^\dagger(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_1 t_1) \right) \\ &= \delta(\mathbf{x}_1 - \mathbf{x}_2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \hat{\psi}_H^\dagger(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_3 t_1) - w(\mathbf{x}_1, \mathbf{x}_3) \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) \hat{\psi}_H(\mathbf{x}_1 t_1) \end{aligned} \quad (5.31)$$

We therefore obtain

$$\begin{aligned} \Sigma^\delta(1, 2) &= \delta(1, 2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \langle \hat{\psi}_H^\dagger(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_3 t_1) \rangle - \delta(t_1, t_2) w(\mathbf{x}_1, \mathbf{x}_2) \langle \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) \hat{\psi}_H(\mathbf{x}_1 t_1) \rangle \\ &= -i\delta(1, 2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) G^<(\mathbf{x}_3 t_1, \mathbf{x}_3 t_1) + i\delta(t_1, t_2) w(\mathbf{x}_1, \mathbf{x}_2) G^<(\mathbf{x}_1 t_1, \mathbf{x}_2 t_1) \end{aligned} \quad (5.32)$$

This expression will later be denoted as the Hartree-Fock form of the self-energy.

In this section we showed that  $\Sigma = \hat{\Sigma}$  and therefore the equations of motion can be written as

$$[i\partial_{t_1} - h(1)] G(1, 2) = \delta(1, 2) + \int d3 \Sigma(1, 3) G(3, 2). \quad (5.33)$$

$$[-i\partial_{t_2} - h(2)] G(1, 2) = \delta(1, 2) + \int d3 G(1, 3) \Sigma(3, 2). \quad (5.34)$$

We see later that if we consider more general initial conditions that  $\Sigma$  is no longer equal to its adjoint  $\hat{\Sigma}$ . The next task is find more explicit forms of the self-energy. The self-energy is a functional of the one-particle Green function, and as a consequence, Eqs. (5.33) and (5.34) constitute a set of equations that should be solved to self-consistency once the functional dependence of  $\Sigma$  on  $G$  is known. This is the topic of the next section.

## 5.2 Derivation of self-consistent equations

To generate a set of self-consistent equations we first note that from Eq.(3.48) it follows that

$$\frac{\delta G(1, 2)}{\delta v(3)} = -i \frac{\delta}{\delta v(3)} \langle T_c[\hat{\psi}_H(1) \hat{\psi}_H^\dagger(2)] \rangle = -\langle T_C[\hat{\psi}_H(1) \hat{\psi}_H^\dagger(2) \hat{n}_H(3)] \rangle + \langle \hat{n}_H(3) \rangle \langle T_C[\hat{\psi}_H(1) \hat{\psi}_H^\dagger(2)] \rangle \quad (5.35)$$

and we can therefore write

$$-i\langle T_C[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)]\rangle = i\frac{\delta G(1,2)}{\delta v(3)} + \langle \hat{n}_H(3) \rangle G(1,2) \quad (5.36)$$

With this expression we can write the equations of motion Eqs.(5.9) and (5.10) as [6]

$$\begin{aligned} [i\partial_{t_1} - h(1)]G(1,1') &= \delta(1,1') \\ &+ i \int d2 w(1^+,2) \frac{\delta G(1,1')}{\delta v(2)} + G(1,1') \int d2 w(1,2) \langle \hat{n}_H(2) \rangle \end{aligned} \quad (5.37)$$

$$\begin{aligned} [-i\partial_{t'_1} - h(1')]G(1,1') &= \delta(1,1') \\ &+ i \int d2 w(1'^+,2) \frac{\delta G(1,1')}{\delta v(2)} + G(1,1') \int d2 w(1',2) \langle \hat{n}_H(2) \rangle \end{aligned} \quad (5.38)$$

As a next step we will derive an expression for  $\delta G(1,1')/\delta v(2)$ . To do this we differentiate the equations of motion Eq.(5.33) and Eq.(5.34) with respect to  $v$  and obtain the equations:

$$(i\partial_{t_1} - h(1))\frac{\delta G(1,1')}{\delta v(2)} - \int d3 \Sigma(1,3) \frac{\delta G(3,1)}{\delta v(2)} = \delta(1,2)G(1,1') + \int d3 \frac{\delta \Sigma(1,3)}{\delta v(2)} G(3,1') \quad (5.39)$$

$$(-i\partial_{t'_1} - h(1'))\frac{\delta G(1,1')}{\delta v(2)} - \int d3 \frac{\delta G(1,3)}{\delta v(2)} \Sigma(3,1') = \delta(1',2)G(1,1') + \int d3 G(1,3) \frac{\delta \Sigma(3,1')}{\delta v(2)} \quad (5.40)$$

From the equation of motion of the Green function we can see that a general solution to these equations is

$$\frac{\delta G(1,1')}{\delta v(2)} = G(1,2)G(2,1') + \int d3 d4 G(1,3) \frac{\delta \Sigma(3,4)}{\delta v(2)} G(4,1') + C(1,1',2) \quad (5.41)$$

where  $C$  is a solution to the homogeneous equations

$$(i\partial_{t_1} - h(1))C(1,1',2) - \int d3 \Sigma(1,3)C(3,1',2) = 0 \quad (5.42)$$

$$(-i\partial_{t'_1} - h(1'))C(1,1',2) - \int d3 C(1,3,2)\Sigma(3,1') = 0 \quad (5.43)$$

---

### Exercise

Check that the expression in Eq.(5.41) is a solution to Eqs.(5.39) and (5.40).

---

To determine the solution uniquely we must use the boundary conditions. Since both terms on the right hand side of Eq.(5.35) satisfy the Kubo-Martin-Schwinger boundary conditions see that

$$\frac{\delta G(\mathbf{x}_1, t_0 - i\beta, 1')}{\delta v(2)} = -\frac{\delta G(\mathbf{x}_1, t_0, 1')}{\delta v(2)} \quad (5.44)$$

$$\frac{\delta G(1, \mathbf{x}'_1, t_0 - i\beta)}{\delta v(2)} = -\frac{\delta G(1, \mathbf{x}'_1, t_0)}{\delta v(2)} \quad (5.45)$$

It is readily seen from the boundary conditions on the Green function that the first two terms in Eq.(5.41) satisfy the boundary conditions Eq.(A.5) and (5.45). Therefore also the function  $C$  must satisfy these boundary conditions. This uniquely fixes  $C = 0$  as the solution to Eqs.(5.42) and (5.43). We thus have

$$\frac{\delta G(1,1')}{\delta v(2)} = G(1,2)G(2,1') + \int d3 d4 G(1,3) \frac{\delta \Sigma(3,4)}{\delta v(2)} G(4,1') \quad (5.46)$$

From the structure of this equation is then natural to define the following so-called vertex function  $\Gamma$  as

$$\Gamma(12; 3) = \delta(1, 2)\delta(2, 3) + \frac{\delta\Sigma(1, 2)}{\delta v(3)} \quad (5.47)$$

such that we have

$$\frac{\delta G(1, 1')}{\delta v(2)} = \int d3 d4 G(1, 3)G(4, 1')\Gamma(34; 2) \quad (5.48)$$

If we insert this equation into Eq.(5.37) we obtain

$$\begin{aligned} & [i\partial_{t_1} - h(1)]G(1, 1') = \delta(1, 1') \\ & + i \int d2 d3 d4 G(1, 3)w(1^+, 2)\Gamma(34; 2)G(4, 1') + G(1, 1') \int d2 w(1, 2)\langle \hat{n}_H(2) \rangle \\ & = \delta(1, 1') + \int d4 \Sigma(1, 4)G(4, 1') \end{aligned} \quad (5.49)$$

We therefore see that we can write  $\Sigma$  as

$$\Sigma(1, 2) = i \int d3 d4 G(1, 3)w(1^+, 4)\Gamma(32; 4) - i\delta(1, 2) \int d3 w(1, 3)G(3, 3^+) \quad (5.50)$$

where we used that  $\langle \hat{n}_H(3) \rangle = -iG(3, 3^+)$ . This equation can be used iteratively to generate expressions for  $\Sigma$  in terms of the Green function. This becomes more clear when we insert into Eq.(5.50) the explicit form of the vertex (5.47) :

$$\begin{aligned} \Sigma(1, 2) & = iG(1, 2)w(1^+, 2) - i\delta(1, 2) \int d3 w(1, 3)G(3, 3^+) \\ & + i \int d3 d4 G(1, 3)w(1^+, 4)\frac{\delta\Sigma(3, 2)}{\delta v(4)} \end{aligned} \quad (5.51)$$

The first line in this expression is defined as the Hartree-Fock self-energy

$$\Sigma^{\text{HF}}[G, w](1, 2) = iG(1, 2)w(1^+, 2) - i\delta(1, 2) \int d3 w(1, 3)G(3, 3^+) \quad (5.52)$$

The first iteration of Eq.(5.51) gives

$$\begin{aligned} \Sigma(1, 2) & = \Sigma^{\text{HF}}(1, 2) + i \int d3 d4 G(1, 3)w(1^+, 4)\frac{\delta\Sigma^{\text{HF}}(3, 2)}{\delta v(4)} \\ & + i^2 \int d3 d4 G(1, 3)w(1^+, 4)\frac{\delta}{\delta v(4)} \int d5 d6 G(3, 5)w(3^+, 6)\frac{\delta\Sigma(5, 2)}{\delta v(6)} \end{aligned} \quad (5.53)$$

We can now evaluate  $\delta\Sigma^{\text{HF}}/\delta v$  using Eq.(5.46):

$$\begin{aligned} \frac{\delta\Sigma^{\text{HF}}(3, 2)}{\delta v(4)} & = i\frac{\delta G(3, 2)}{\delta v(4)}w(3^+, 2) - i\delta(3, 2) \int d5 w(3, 5)\frac{\delta G(5, 5^+)}{\delta v(4)} \\ & = iG(3, 4)G(4, 2)w(3^+, 2) - i\delta(3, 2) \int d5 w(3, 5)G(5, 4)G(4, 5^+) \\ & - i\delta(3, 2) \int d5 d6 d7 w(3, 5)G(5, 6)\frac{\delta\Sigma(6, 7)}{\delta v(4)}G(7, 5^+) \\ & + iw(3^+, 2) \int d5 d6 d7 G(3, 6)\frac{\delta\Sigma(6, 7)}{\delta v(4)}G(7, 2) \end{aligned} \quad (5.54)$$



Figure 5.1: Diagrammatic expression of  $\Sigma^{(2)}$

When we insert this expression back into Eq.(5.53) we obtain

$$\begin{aligned}
\Sigma(1,2) &= \Sigma^{(2)}(1,2) - i^2 \int d4d6d7 G(1,2)w(1^+,4)w(2,5)G(5,6) \frac{\delta\Sigma(6,7)}{\delta v(4)} G(7,5^+) \\
&+ i^2 \int d3d4d6d7 G(1,3)w(1,4^+)w(3,2^+)G(3,6) \frac{\delta\Sigma(6,7)}{\delta v(4)} G(7,2) \\
&+ i^2 \int d3d4 G(1,3)w(1^+,4) \frac{\delta}{\delta v(4)} \int d5d6 G(3,5)w(3^+,6) \frac{\delta\Sigma(5,2)}{\delta v(6)} \quad (5.55)
\end{aligned}$$

where we defined  $\Sigma^{(2)}$  as

$$\begin{aligned}
\Sigma^{(2)}[G,w](1,2) &= \Sigma^{\text{HF}}(1,2) + i^2 \int d3d4 G(1,3)w(1^+,4)G(3,4)G(4,2)w(3^+,2) \\
&- i^2 \int d4d5 G(1,2)w(1^+,4)w(2,5)G(5,4)G(4,5^+) \quad (5.56)
\end{aligned}$$

We see that  $\Sigma^{(2)}$  for a given  $G$  and as functional of  $w$  is of second order in  $w$ . This term can be represented diagrammatically. To do this we associate with every Green function  $G(1,2)$  a directed line running from 2 to 1 and with every interaction line  $w(1,2)$  a wiggly line connecting point 1 and 2. This is illustrated in Fig. 5.1 for the expression given in Eq.(5.56). The remaining terms in Eq.(5.55) that contain derivatives of  $\Sigma$  are of higher order in  $w$ . For instance a further iteration of Eq.(5.55) produces new terms that are of third order in  $w$ . The main message is that we have found a systematic way of expressing the self-energy  $\Sigma$  as a functional of  $G$  and  $w$ . The whole iterative set of equations be written compactly by writing a coupled equation for the self-energy  $\Sigma$  and the vertex  $\Gamma$ . If we regard  $\Sigma$  as a functional of the Green function Eq.(5.47) implies immediately that

$$\begin{aligned}
\Gamma(12;3) &= \delta(1,2)\delta(1,3) + \int d4d5 \frac{\delta\Sigma(1,2)}{\delta G(4,5)} \frac{\delta G(4,5)}{\delta v(3)} \\
&= \delta(1,2)\delta(1,3) + \int d4d5d6d7 \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\Gamma(67;3) \quad (5.57)
\end{aligned}$$

We have therefore obtained the following set of self-consistent equations

$$0 = [i\partial_{t_1} - h(1)] G(1,1') - \delta(1,1') - \int d2 \Sigma(1,2)G(2,1') \quad (5.58)$$

$$0 = [-i\partial_{t_1} - h(1')] G(1,1') - \delta(1,1') - \int d2 G(1,2)\Sigma(2,1') \quad (5.59)$$

$$\Sigma(1,2) = i \int d3d4 G(1,3)w(1^+,4)\Gamma(32;4) - i\delta(1,2) \int d3 w(1,3)G(3,3^+) \quad (5.60)$$

$$\Gamma(12;3) = \delta(1,2)\delta(1,3) + \int d4d5d6d7 \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\Gamma(67;3) \quad (5.61)$$

These equations can now be iterated to obtain self-consistent equations for the Green function. For instance, if we take the simplest approximation for the vertex, namely  $\Gamma(12; 3) = \delta(1, 2)\delta(1, 3)$ , and insert it into Eq.(5.60) we obtain the Hartree-Fock approximation to the self-energy  $\Sigma^{HF}$ . By inserting this expression into Eq.(5.61) we obtain a new approximation for the vertex from which one can obtain a new self-energy. As one can readily convince oneself the time-local part (i.e. proportional to  $\delta(t_1, t_2)$ ) of  $\Sigma$  is only given by  $\Sigma^{HF}$ , i.e.  $\Sigma^\delta = \Sigma^{HF}$ . It is therefore convenient to single out the Hartree-Fock part of the self-energy, such that [2]

$$\Sigma(1, 2) = \Sigma^{HF}(1, 2) + \theta(t_1, t_2)\Sigma^>(1, 2) + \theta(t_2, t_1)\Sigma^<(1, 2) \quad (5.62)$$

From expression (5.52) we see that we can write

$$\Sigma^{HF}(1, 2) = \Sigma^{HF}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_1)\delta(t_1, t_2) \quad (5.63)$$

where

$$\Sigma^{HF}(\mathbf{x}_1, t_1, \mathbf{x}_2 t_1) = iG^<(\mathbf{x}_1 t_1, \mathbf{x}_2 t_1)w(\mathbf{x}_1, \mathbf{x}_2) - i\delta(\mathbf{x}_1 - \mathbf{x}_2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3)G^<(\mathbf{x}_3 t_1, \mathbf{x}_3 t_1) \quad (5.64)$$

Some specific forms for the self-energy will be discussed later. Let us first discuss the form of the equations of motion that one has to solve in any practical application.

### 5.3 The Kadanoff-Baym equations

Using Eq.(5.62) we transform the contour integration to obtain:

$$(i\partial_{t_1} - h(1))G^{\lessdot}(1, 2) = I_1^{\lessdot}(1, 2) \quad (5.65)$$

$$(-i\partial_{t_2} - h(2))G^{\lessdot}(1, 2) = I_2^{\lessdot}(1, 2) \quad (5.66)$$

$$(i\partial_{t_1} - h(1))G^{\lrcorner}(1, 2) = I^{\lrcorner}(1, 2) \quad (5.67)$$

$$(-i\partial_{t_2} - h(2))G^{\lrcorner}(1, 2) = I^{\lrcorner}(1, 2) \quad (5.68)$$

$$(-\partial_{\tau_1} - h(1))G^{\text{M}}(1, 2) = i\delta(\tau_1 - \tau_2) + I^{\text{M}}(1, 2) \quad (5.69)$$

$$(\partial_{\tau_2} - h(2))G^{\text{M}}(1, 2) = i\delta(\tau_1 - \tau_2) + I^{\text{M}}(1, 2) \quad (5.70)$$

where we defined the collision terms

$$I_1^{\lessdot} = (\Sigma G)^{\lessdot} = \Sigma^{\text{R}} \cdot G^{\lessdot} + \Sigma^{\lessdot} \cdot G^{\text{A}} + \Sigma^{\lrcorner} \star G^{\lrcorner} \quad (5.71)$$

$$I_2^{\lessdot} = (G\Sigma)^{\lessdot} = G^{\text{R}} \cdot \Sigma^{\lessdot} + G^{\lessdot} \cdot \Sigma^{\text{A}} + G^{\lrcorner} \star \Sigma^{\lrcorner} \quad (5.72)$$

$$I^{\lrcorner} = (\Sigma G)^{\lrcorner} = \Sigma^{\text{R}} \cdot G^{\lrcorner} + \Sigma^{\lrcorner} \star G^{\text{M}} \quad (5.73)$$

$$I^{\lrcorner} = (G\Sigma)^{\lrcorner} = G^{\lrcorner} \cdot \Sigma^{\text{A}} + G^{\text{M}} \star \Sigma^{\lrcorner} \quad (5.74)$$

$$I^{\text{M}} = (\Sigma G)^{\text{M}} = \Sigma^{\text{M}} \star G^{\text{M}} \quad (5.75)$$

The Eqs. (5.65) to (5.70) are known as the Kadanoff-Baym equations [7, 5, 8]. For a given approximation of  $\Sigma[G]$  these equations can be solved by time-propagation. In practice the equations are first solved for  $G^{\text{M}}$  on the contour from  $t_0$  to  $t_0 - i\beta$  parallel to the imaginary axis using the Kubo-Martin-Schwinger boundary conditions [9, 10, 11]. This amounts to a solution of the stationary equilibrium problem. In fact since the Green function on the vertical part of the contour

corresponds to an equilibrium situation and only depends on  $\tau = \tau_1 - \tau_2$  the Eqs.(5.69) and (5.70) can be replaced by a single equation

$$(-\partial_\tau - h(1))G^M(\mathbf{x}_1, \mathbf{x}_2; \tau) = i\delta(\tau) + I^M(\mathbf{x}_1, \mathbf{x}_2, \tau) \quad (5.76)$$

where we defined

$$G^M(\mathbf{x}_1, \mathbf{x}_2; \tau_1 - \tau_2) = G^M(\mathbf{x}_1\tau_1, \mathbf{x}_2\tau_2) \quad (5.77)$$

The functions such obtained can then be used as starting values for the real time propagation of the functions  $G^{\lessgtr}, G^\lceil$  and  $G^\lrcorner$ . The initial conditions for these functions are then given by

$$G^\lrcorner(t_0, \tau) = G^M(0, \tau) \quad (5.78)$$

$$G^\lceil(\tau, t_0) = G^M(\tau, 0) \quad (5.79)$$

$$G^<(t_0, t_0) = G^M(0, 0^+) \quad (5.80)$$

$$G^>(t_0, t_0) = G^M(0^+, 0) \quad (5.81)$$

---

### Exercise

Derive the form of the Kadanoff-Baym equations given in Eqns.(5.65) to Eqns.(5.69) from the equation of motion on the contour and check the initial conditions Eq.(8.12) to Eq.(5.81).

---

The solution of the equations of motion is further simplified by the relations

$$[G^{\lessgtr}(1, 2)]^* = -G^{\lessgtr}(2, 1) \quad (5.82)$$

$$G^>(\mathbf{x}_1 t, \mathbf{x}_2 t) = -i\delta(\mathbf{x}_1 - \mathbf{x}_2) + G^<(\mathbf{x}_1 t, \mathbf{x}_2 t) \quad (5.83)$$

This means that in the time propagation one can restrict oneself to solving  $G^>(1, 2)$  for  $t_1 > t_2$  and  $G^<(1, 2)$  for  $t_2 \leq t_1$ .

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### Exercise

Prove relations (5.82) and (5.83)

---

Let now discuss some physical properties that are contained in these equations of motion. As an example we write out Eq.(5.65) out in more detail. We then have

$$\begin{aligned} (i\partial_{t_1} - h(1))G^<(1, 2) &= \int d\mathbf{x}_3 \Sigma^{\text{HF}}(\mathbf{x}_1 t_1, \mathbf{x}_3 t_1) G^<(\mathbf{x}_3 t_1, 2) \\ &+ \int_{t_0}^{t_1} d3 [\Sigma^>(1, 3) - \Sigma^<(1, 3)] G^<(3, 2) - \int_{t_0}^{t_2} d3 \Sigma^<(1, 3) [G^>(3, 2) - G^<(3, 2)] \\ &- i \int_0^\beta d3 G^\lceil(1, 3) \Sigma^\lrcorner(3, 2) \end{aligned} \quad (5.84)$$

The Hartree-Fock term on the right hand side of the equation is a potential that is spatially nonlocal, but local in time. Consequently it has no memory and does not lead to dissipation. The next to terms on the other hand involve time-integrations over all previous times. The complex self-energy kernels in these equations lead to dephasing and dissipative effects in the Green functions and lead to a decay of the Green function far from the time-diagonal. The last term on the right hand side is (apart from the Hartree-Fock term) the only term that remains for  $t_1 = t_2 = t_0$ . It therefore describes the initial correlations in the system.

## Chapter 6

# Conserving approximations

### 6.1 Conservation laws and $\Phi$ -derivability

There are several general exact relations known for systems in time-dependent external fields. These relations reduce in absence of the external field to the conservation laws for energy, momentum, angular momentum and particle number. The main question is now whether these conservation laws are also obeyed if we calculate the energy, momentum and angular momentum from the Green function obtained within a certain approximation. Approximations that do conserve them will be denoted as conserving approximations. The main question is then: how can we guarantee that a given approximation to the self-energy gives a conserving approximation for the Green function. Let us first discuss a number of conservation laws. If we know the Green function we can calculate the density and the current density from

$$\langle \hat{n}(1) \rangle = -iG(1, 1^+) \quad (6.1)$$

$$\langle \mathbf{j}(1) \rangle = -i \left\{ \left[ \frac{\nabla_1}{2i} - \frac{\nabla_{1'}}{2i} + \mathbf{A}(1) \right] G(1, 1') \right\}_{1'=1^+} \quad (6.2)$$

An important relation between the two quantities is provided by the continuity equation:

$$\partial_{t_1} \langle \hat{n}(1) \rangle + \nabla \cdot \langle \mathbf{j}(1) \rangle = 0 \quad (6.3)$$

This relation tells us that accumulation of charge in a certain region of space is related to current flow into that region. This is certainly an important relation that one wants to have satisfied in the analysis of charge transport processes. If we know the current density we can further calculate the total momentum and angular momentum expectation values in the system from the equations

$$\langle \mathbf{P}(t_1) \rangle = \int d\mathbf{x}_1 \langle \mathbf{j}(1) \rangle \quad (6.4)$$

$$\langle \mathbf{L}(t_1) \rangle = \int d\mathbf{x}_1 \mathbf{r}_1 \times \langle \mathbf{j}(1) \rangle \quad (6.5)$$



For these two quantities the following relations should be satisfied

$$\partial_{t_1} \langle \mathbf{P}(t_1) \rangle = - \int d\mathbf{x}_1 \left[ \langle \hat{n}(1) \rangle \mathbf{E}(1) + \langle \mathbf{j}(1) \rangle \times \mathbf{B}(1) \right] \quad (6.6)$$

$$\partial_{t_1} \langle \mathbf{L}(t_1) \rangle = - \int d\mathbf{x}_1 \left[ \langle \hat{n}(1) \rangle \mathbf{r}_1 \times \mathbf{E}(1) + \mathbf{r}_1 \times (\langle \mathbf{j}(1) \rangle \times \mathbf{B}(1)) \right] \quad (6.7)$$

where  $\mathbf{E}$  and  $\mathbf{B}$  are the electric and magnetic fields calculated from

$$\mathbf{E}(1) = \nabla_1 v(1) - \partial_{t_1} \mathbf{A}(1) \quad (6.8)$$

$$\mathbf{B}(1) = \nabla_1 \times \mathbf{A}(1) \quad (6.9)$$

The equations (6.6) and (6.7) tell us that the change in momentum and angular momentum is equal to the total force and total torque on the system. In the absence of external fields these equations express momentum and angular momentum conservation. Since the right hand sides of Eq.(6.6) and Eq.(6.7) can also directly be calculated from the density and the current and therefore from the Green function, we may wonder whether they are satisfied for a given approximation to the Green function. Finally we will consider the case of energy conservation. Let  $E(t_1) = \langle \hat{H}(t_1) \rangle$  be the energy expectation value of the system, then we have

$$\partial_{t_1} E(t_1) = - \int d\mathbf{x}_1 \langle \mathbf{j}(1) \rangle \cdot \mathbf{E}(1) \quad (6.10)$$

This equation tells us that the energy change of the system is equal to the work done on the system. Again we can ask whether this equation is satisfied for a given approximation to Green function. Let us first explain how the energy is calculated from the Green function. First of all, the one-particle energy is simply calculated from

$$\langle h(1) \rangle = -i \int d\mathbf{x}_1 h(1') G(1, 1') \Big|_{1'=1^+} = -i \int d\mathbf{x}_1 h(\mathbf{x}_1, t_1) G^<(\mathbf{x}_1 t_1, \mathbf{x}'_1 t_1) \Big|_{\mathbf{x}'_1 = \mathbf{x}_1} \quad (6.11)$$

To calculate the expectation value of the interaction energy we simply use Eq.(5.1) to obtain

$$i \partial_{t_1} G^<(1, 2) = h(1) G^<(1, 2) + i \int d3 w(1, 3) \langle \hat{\psi}_H^\dagger(2) \hat{\psi}_H^\dagger(3) \hat{\psi}_H(3) \hat{\psi}_H(1) \rangle \quad (6.12)$$

and therefore

$$(i \partial_{t_1} - h(1)) G^<(1, 2) \Big|_{t_2=t_1} = \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \langle \hat{\psi}_H^\dagger(\mathbf{x}_2 t_1) \hat{\psi}_H^\dagger(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_3 t_1) \hat{\psi}_H(\mathbf{x}_1 t_1) \rangle = 2i \langle \hat{W}(t_1) \rangle \quad (6.13)$$

We then obtain for the total energy the expression

$$E(t_1) = \langle h(t_1) \rangle + \langle \hat{W}(t_1) \rangle = -\frac{i}{2} \int d\mathbf{x}_1 (i \partial_{t_1} + h(\mathbf{x}_1, t_1)) G^<(\mathbf{x}_1 t_1, \mathbf{x}'_1 t_1) \Big|_{\mathbf{x}'_1 = \mathbf{x}_1} \quad (6.14)$$

The question is now whether with this energy calculated from an approximate Green function and with the current density calculated from the same Green function relation (6.10) is satisfied. These questions were answered by Baym [12] in a famous paper. The main conclusion of the paper is as follows : If the self-energy  $\Sigma$  is obtained from an underlying functional  $\Phi[G]$ , according to

$$\Sigma(1, 2) = \frac{\delta \Phi}{\delta G(2, 1)}, \quad (6.15)$$

$$\begin{aligned}
\Phi &= -\frac{1}{2} \text{diagram}_1 - \frac{1}{2} \text{diagram}_2 - \frac{1}{4} \text{diagram}_3 - \frac{1}{4} \text{diagram}_4 \\
&\quad - \frac{1}{6} \text{diagram}_5 - \frac{1}{6} \text{diagram}_6 - \frac{3}{6} \text{diagram}_7 + \dots \\
-i\Sigma &= \text{diagram}_8 + \text{diagram}_9 + \text{diagram}_{10} + \text{diagram}_{11} + \text{diagram}_{12} \\
&\quad + \text{diagram}_{13} + \text{diagram}_{14} + \text{diagram}_{15} + \text{diagram}_{16} + \dots
\end{aligned}$$

Figure 6.1: Some of the low-order  $\Phi$  diagrams, and some of the self-energy diagrams obtained from  $\Sigma = \delta\Phi/\delta G$ . The prefactor of a  $\Phi$ -diagram is  $n_\Sigma/2n$  where  $n_\Sigma$  is the number of topologically different  $\Sigma$ -diagrams that can be generated from it and  $n$  is the number of interaction lines.

then solving the Kadanoff-Baym equations with this approximation to the self-energy will lead to a Green function  $G$  that satisfies exactly the relations (6.3), (6.6), (6.7) and (6.10). The question is now how the functional  $\Phi$  can be constructed. Such a functional  $\Phi$  can be constructed, as first shown by Luttinger and Ward [13], by summing over irreducible self-energy diagrams closed with an additional Green function line and multiplied by appropriate numerical factors,

$$\Phi[G] = \sum_{n,k} \frac{1}{2n} \int d1d2 \Sigma_k^{(n)}(1,2)G(2,1^+) = \sum_{n,k} \frac{1}{2n} \text{tr} \left[ \Sigma_k^{(n)} G \right]. \quad (6.16)$$

The term  $n$  indicates the number of interaction lines and  $k$  labels  $\Sigma$ -diagrams. The trace  $\text{tr}$  indicates an integration over all variables (in contrast to the trace  $\text{Tr}$  that denotes a summation over a complete set of states in the Hilbert space). Some of the low-order diagrams are shown in Fig. 6.1, together with some of the corresponding self-energy diagrams.

## 6.2 Approximate conserving schemes

### 6.2.1 Time-dependent Hartree-Fock approximation

We now consider some approximate conserving schemes. One of the simplest approximations we can take is the Hartree-Fock approximation for  $\Sigma$ . For this approximation the  $\Phi$ -diagrams correspond to the first two in Fig.6.1 and the self-energy is explicitly given by Eq.(5.52) or in more detail in

Eqs.(5.63) and (5.64) In that case the equations of motion for  $G^{\lessgtr}$  are given by

$$(i\partial_{t_1} - h(1))G^{\lessgtr}(1, 2) = \int d\mathbf{x}_3 \Sigma^{\text{HF}}(1, \mathbf{x}_3 t_1) G^{\lessgtr}(\mathbf{x}_3 t_1, 2) \quad (6.17)$$

$$(-i\partial_{t_2} - h(2))G^{\lessgtr}(1, 2) = \int d\mathbf{x}_3 G^{\lessgtr}(1, \mathbf{x}_3 t_2) \Sigma^{\text{HF}}(\mathbf{x}_3 t_2, 2) \quad (6.18)$$

To solve these equations we first introduce the following orbitals

$$(i\partial_{t_1} - h(1))\varphi_i(1) = \int d\mathbf{x}_3 \Sigma^{\text{HF}}(1, \mathbf{x}_3 t_1) \varphi_i(\mathbf{x}_3 t_1) \quad (6.19)$$

$$(-i\partial_{t_2} - h(2))\bar{\varphi}_i(2) = \int d\mathbf{x}_3 \bar{\varphi}_i(\mathbf{x}_3 t_2) \Sigma^{\text{HF}}(\mathbf{x}_3 t_2, 2) \quad (6.20)$$

From the basic property (5.82) and the explicit form of  $\Sigma^{\text{HF}}$  of Eq.(5.64) it follows that  $\Sigma^{\text{HF}}$  is hermitian and therefore  $\bar{\varphi}_i = \varphi_i^*$  (this is not true anymore on the vertical part of the contour). We now make the following Ansatz for  $G^<$  :

$$G^<(1, 2) = i \sum_j n_j \varphi_j(1) \varphi_j^*(2) \quad (6.21)$$

where  $n_j$  are constants to be determined. It is clear that this Ansatz for  $G^<$  satisfies Eqs.(6.17) and (6.18) but we still need to check the boundary conditions. In order to satisfy Eq.(5.83) we make for  $G^>$  the Ansatz

$$G^>(1, 2) = -i \sum_j (1 - n_j) \varphi_j(1) \varphi_j^*(2) \quad (6.22)$$

such that

$$G^>(1, 2) \Big|_{t_1=t_2} - G^<(1, 2) \Big|_{t_1=t_2} = -i \sum_j \varphi_j(1) \varphi_j^*(2) \Big|_{t_1=t_2} = -i \delta(\mathbf{x}_1 - \mathbf{x}_2) \quad (6.23)$$

We must further specify the initial conditions. This can be done with help of Eqs.(5.80) and (5.81). We therefore first have to solve for the Green function  $G^{\text{M}}$  on the imaginary part of the contour where  $t = -i\tau$  as given in Eq.(4.13).

$$G^{\text{M}}(\mathbf{x}_1 \tau_1, \mathbf{x}_2 \tau_2) = \theta(\tau_1 - \tau_2) G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) + \theta(\tau_2 - \tau_1) G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) \quad (6.24)$$

If we define  $\chi_i(\mathbf{x}_1 \tau_1) = \varphi_i(\mathbf{x}_1, -i\tau_1)$  and  $\bar{\chi}_i(\mathbf{x}_1 \tau_1) = \varphi_i^*(\mathbf{x}_1, -i\tau_1)$  then we have

$$G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = -i \sum_j (1 - n_j) \chi_j(\mathbf{x}_1 \tau_1) \bar{\chi}_j(\mathbf{x}_2 \tau_2) \quad (6.25)$$

$$G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = i \sum_j n_j \chi_j(\mathbf{x}_1 \tau_1) \bar{\chi}_j(\mathbf{x}_2 \tau_2) \quad (6.26)$$

where  $\chi_i$  and  $\bar{\chi}_i$  satisfy the equations

$$(-\partial_{\tau_1} - h(\mathbf{x}_1))\chi_i(\mathbf{x}_1 \tau_1) = \int d\mathbf{x}_3 \Sigma^{\text{HF}}(\mathbf{x}_1 \tau_1, \mathbf{x}_3 \tau_1) \chi_i(\mathbf{x}_3 \tau_1) \quad (6.27)$$

$$(\partial_{\tau_2} - h(\mathbf{x}_2))\bar{\chi}_i(\mathbf{x}_2 \tau_2) = \int d\mathbf{x}_3 \bar{\chi}_i(\mathbf{x}_3 \tau_2) \Sigma^{\text{HF}}(\mathbf{x}_3 \tau_2, \mathbf{x}_2 \tau_2) \quad (6.28)$$

With these equations it is readily seen that the equations of motion for  $G^M$  of (5.70) and (5.76) are indeed satisfied. We therefore only have to specify the boundary condition. On the vertical contour the system is in equilibrium and therefore  $\Sigma^{\text{HF}}(\mathbf{x}_1\tau, \mathbf{x}_2\tau)$  does not depend on  $\tau$ . For the functions  $\chi_i$  and  $\bar{\chi}_i$  we can therefore make the Ansatz

$$\chi_i(\mathbf{x}_1\tau_1) = \psi_i(\mathbf{x}_1)e^{-\epsilon_i\tau_1} \quad (6.29)$$

$$\bar{\chi}_i(\mathbf{x}_1\tau_1) = \psi_i^*(\mathbf{x}_1)e^{\epsilon_i\tau_1} \quad (6.30)$$

If we insert these forms in Eq.(6.27) and (6.28) we obtain

$$(\epsilon_i - h(\mathbf{x}_1))\psi_i(\mathbf{x}_1) = \int d\mathbf{x}_3 \Sigma^{\text{HF}}(\mathbf{x}_1\tau_1, \mathbf{x}_3\tau_1)\psi_i(\mathbf{x}_3) \quad (6.31)$$

$$(\epsilon_i - h(\mathbf{x}_2))\psi_i^*(\mathbf{x}_2\tau_2) = \int d\mathbf{x}_3 \psi_i^*(\mathbf{x}_3)\Sigma^{\text{HF}}(\mathbf{x}_3\tau_2, \mathbf{x}_2\tau_2) \quad (6.32)$$

and we obtain

$$G^>(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = -i \sum_j (1 - n_j) e^{-\epsilon_i(\tau_1 - \tau_2)} \psi_j(\mathbf{x}_1) \psi_j^*(\mathbf{x}_2) \quad (6.33)$$

$$G^<(\mathbf{x}_1, -i\tau_1, \mathbf{x}_2, -i\tau_2) = i \sum_j n_j e^{-\epsilon_i(\tau_1 - \tau_2)} \psi_j(\mathbf{x}_1) \psi_j^*(\mathbf{x}_2) \quad (6.34)$$

From these equations and Eq.(5.64) we see indeed that on the imaginary part of the contour the self-energy is time-independent and given by

$$\Sigma^{\text{HF}}(\mathbf{x}_1, \mathbf{x}_2) = -w(\mathbf{x}_1, \mathbf{x}_2) \sum_j n_j \psi_j(\mathbf{x}_1) \psi_j^*(\mathbf{x}_2) + \delta(\mathbf{x}_1 - \mathbf{x}_2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \sum_j n_j \psi_j(\mathbf{x}_3) \psi_j^*(\mathbf{x}_3) \quad (6.35)$$

Let us now determine the coefficients  $n_j$  from the Kubo-Martin-Schwinger boundary conditions. From condition Eq.(4.18) and the explicit forms (6.33) and (6.34) we see that we must have

$$\begin{aligned} G^<(\mathbf{x}_1, 0, \mathbf{x}_2, -i\tau_2) &= i \sum_j n_j e^{\epsilon_i\tau_2} \psi_j(\mathbf{x}_1) \psi_j^*(\mathbf{x}_2) \\ &= i \sum_j (1 - n_j) e^{-\epsilon_i(\beta - \tau_2)} \psi_j(\mathbf{x}_1) \psi_j^*(\mathbf{x}_2) = -G^>(\mathbf{x}_1, -i\beta, \mathbf{x}_2, \tau_2) \end{aligned} \quad (6.36)$$

We thus obtain the relation

$$n_j = (1 - n_j) e^{-\epsilon_j\beta} \quad (6.37)$$

this equation is easily solve to give

$$n_j = \frac{1}{e^{\beta\epsilon_j} + 1} \quad (6.38)$$

which is the famous Fermi-Dirac distribution. We have now also completely determined the initial conditions of the orbitals  $\varphi$ , we have  $\varphi_i(\mathbf{x}0) = \psi_i(\mathbf{x})$  where  $\psi_i$  solves Eq.(6.31) with self-energy (6.35). Now that we have completely determined  $G^{\lessgtr}$  we can also explicitly evaluate the self-energy

of Eq.(5.64). The results are summarized below:

$$G^<(1, 2) = i \sum_j n_j \varphi_j(1) \varphi_j^*(2) \quad (6.39)$$

$$G^>(1, 2) = -i \sum_j (1 - n_j) \varphi_j(1) \varphi_j^*(2) \quad (6.40)$$

$$(i\partial_{t_1} - h(1))\varphi_i(1) = \int d\mathbf{x}_3 \Sigma^{\text{HF}}(1, \mathbf{x}_3 t_1) \varphi_i(\mathbf{x}_3 t_1) \quad (6.41)$$

$$\begin{aligned} \Sigma^{\text{HF}}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_1) &= -w(\mathbf{x}_1, \mathbf{x}_2) \sum_j n_j \varphi_i(\mathbf{x}_1 t_1) \varphi_i^*(\mathbf{x}_2 t_1) \\ &+ \delta(\mathbf{x}_1 - \mathbf{x}_2) \int d\mathbf{x}_3 w(\mathbf{x}_1, \mathbf{x}_3) \sum_j n_j \varphi_j(\mathbf{x}_3 t_1) \varphi_j^*(\mathbf{x}_2 t_1) \end{aligned} \quad (6.42)$$

These equations are just the time-dependent Hartree-Fock (TDHF) equations. If we choose the chemical potential  $\mu$  between the highest occupied and lowest unoccupied level of the stationary Hartree-Fock equations and take the zero temperature limit we find that  $n_j$  becomes equal to one for the occupied states and zero for the unoccupied states.

It is now also interesting to see what the time-dependent Hartree-Fock approximation will give for the density response function. From Eq.(5.48) we see that the first order change in the Green function due to a change in the external field is given by

$$\delta G(1, 1') = \int d3d4 G(1, 3)G(4, 1')\Gamma(34; 2)\delta v(2) \quad (6.43)$$

and therefore the density response is given by

$$\delta n(1) = -iG(1, 1^+) = -i \int d3d4 G(1, 3)G(4, 1)\Gamma(34; 2)\delta v(2) = \int d2 \chi(1, 2)\delta v(2) \quad (6.44)$$

and the density response function has the expression

$$\chi(1, 2) = -i \int d3d4 G(1, 3)G(4, 1)\Gamma(34; 2) \quad (6.45)$$

The density response function corresponding to TDHF is then obtained by inserting the vertex function  $\Gamma$  that belongs to TDHF. This function is then the solution of Eq.(5.61) where we need to insert  $\delta\Sigma^{\text{HF}}(1, 2)/\delta G(4, 5)$  for the kernel. We have

$$\frac{\delta\Sigma^{\text{HF}}(1, 2)}{\delta G(4, 5)} = iw(1^+, 2)\delta(1, 4)\delta(2, 5) - i\delta(1, 2)\delta(4, 5^+)w(1, 4) \quad (6.46)$$

and therefore from Eq.(5.61) we obtain

$$\begin{aligned} \Gamma(12; 3) &= \delta(1, 2)\delta(1, 3) + iw(1, 2) \int d6d7 G(1, 6)G(7, 2)\Gamma(67; 3) \\ &- i\delta(1, 2) \int d5d6d7 w(1, 5)G(5, 6)G(7, 5)\Gamma(67; 3) \end{aligned} \quad (6.47)$$

This gives indeed the well-known 'ladder and bubbles' series for the TDHF response function.

## 6.2.2 Second Born approximation

The level conserving approximation contains the second order diagrams, corresponding to the first four  $\Phi$ -diagrams of Fig.6.1 This corresponds to the so-called second Born approximation. Let the second order diagrams be denoted by  $\Sigma^B$  then their explicit form is given by the last two terms of Eq.(5.56), i.e.

$$\Sigma(1, 2) = \Sigma^{\text{HF}}(1, 2) + \Sigma^B(1, 2) \quad (6.48)$$

$$\begin{aligned} \Sigma^B(1, 2) &= i^2 \int d3d4 G(1, 3)w(1^+, 4)G(3, 4)G(4, 2)w(3^+, 2) \\ &\quad - i^2 \int d3d4 G(1, 2)w(1^+, 3)w(2, 4)G(4, 3)G(3, 4^+) \end{aligned} \quad (6.49)$$

Because of the time delta functions contained in  $w(1, 2)$  we can write  $\Sigma^B$  as

$$\begin{aligned} \Sigma^B(1, 2) &= i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G(\mathbf{x}_1 t_1, \mathbf{x}_3 t_2)w(\mathbf{x}_1, \mathbf{x}_4)G(\mathbf{x}_3 t_2, \mathbf{x}_4 t_1)G(\mathbf{x}_4 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_3, \mathbf{x}_2) \\ &\quad - i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_1, \mathbf{x}_3)w(\mathbf{x}_2, \mathbf{x}_4)G(\mathbf{x}_4 t_2, \mathbf{x}_3 t_1)G(\mathbf{x}_3 t_1, \mathbf{x}_4 t_2) \end{aligned} \quad (6.50)$$

We see that these expressions do not involve any time integrations. Therefore it is straightforward to find the various  $\Sigma^x$ -components of this expression where for  $x$  we have  $>, <, \lceil, \rceil, M$ . We have

$$\begin{aligned} \Sigma^{B, \leq}(1, 2) &= i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\leq}(\mathbf{x}_1 t_1, \mathbf{x}_3 t_2)w(\mathbf{x}_1, \mathbf{x}_4)G^{\geq}(\mathbf{x}_3 t_2, \mathbf{x}_4 t_1)G^{\leq}(\mathbf{x}_4 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_3, \mathbf{x}_2) \\ &\quad - i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\leq}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_1, \mathbf{x}_3)w(\mathbf{x}_2, \mathbf{x}_4)G^{\geq}(\mathbf{x}_4 t_2, \mathbf{x}_3 t_1)G^{\leq}(\mathbf{x}_3 t_1, \mathbf{x}_4 t_2) \end{aligned} \quad (6.51)$$

$$\begin{aligned} \Sigma^{B, \lceil}(1, 2) &= i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\lceil}(\mathbf{x}_1 t_1, \mathbf{x}_3 t_2)w(\mathbf{x}_1, \mathbf{x}_4)G^{\lceil}(\mathbf{x}_3 t_2, \mathbf{x}_4 t_1)G^{\lceil}(\mathbf{x}_4 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_3, \mathbf{x}_2) \\ &\quad - i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\lceil}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_1, \mathbf{x}_3)w(\mathbf{x}_2, \mathbf{x}_4)G^{\lceil}(\mathbf{x}_4 t_2, \mathbf{x}_3 t_1)G^{\lceil}(\mathbf{x}_3 t_1, \mathbf{x}_4 t_2) \end{aligned} \quad (6.52)$$

$$\begin{aligned} \Sigma^{B, \rceil}(1, 2) &= i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\rceil}(\mathbf{x}_1 t_1, \mathbf{x}_3 t_2)w(\mathbf{x}_1, \mathbf{x}_4)G^{\rceil}(\mathbf{x}_3 t_2, \mathbf{x}_4 t_1)G^{\rceil}(\mathbf{x}_4 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_3, \mathbf{x}_2) \\ &\quad - i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^{\rceil}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_1, \mathbf{x}_3)w(\mathbf{x}_2, \mathbf{x}_4)G^{\rceil}(\mathbf{x}_4 t_2, \mathbf{x}_3 t_1)G^{\rceil}(\mathbf{x}_3 t_1, \mathbf{x}_4 t_2) \end{aligned} \quad (6.53)$$

$$\begin{aligned} \Sigma^{B, M}(1, 2) &= i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^M(\mathbf{x}_1 t_1, \mathbf{x}_3 t_2)w(\mathbf{x}_1, \mathbf{x}_4)G^M(\mathbf{x}_3 t_2, \mathbf{x}_4 t_1)G^M(\mathbf{x}_4 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_3, \mathbf{x}_2) \\ &\quad - i^2 \int d\mathbf{x}_3 d\mathbf{x}_4 G^M(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2)w(\mathbf{x}_1, \mathbf{x}_3)w(\mathbf{x}_2, \mathbf{x}_4)G^M(\mathbf{x}_4 t_2, \mathbf{x}_3 t_1)G^M(\mathbf{x}_3 t_1, \mathbf{x}_4 t_2) \end{aligned} \quad (6.54)$$

With these expressions and the Kadanoff-Baym equations the problem is completely defined.

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### Exercise

Suppose we calculate the first order density change by propagation of the Kadanoff-Baym equations within the second Born approximation. What would be the diagrammatic structure of the response function that we obtain in this way ?

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### 6.3 Applications

In this section we will illustrate the methods discussed so far with some results. When one does actual calculations the Green functions are often expressed in a basis, i.e. one writes

$$G(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2) = \sum_{i,j} \varphi_i(\mathbf{x}_1) \varphi_j^*(\mathbf{x}_2) G_{ij}(t_1, t_2) \quad (6.55)$$

where  $\varphi_i$  represents a suitable chosen basis such as Hartree-Fock molecular orbitals. The coefficients  $G_{ij}$  are in fact the Green functions with respect the annihilation and creation operators  $\hat{a}_i$  and  $\hat{a}_i^\dagger$  with respect to this basis

$$G_{ij}(t_1, t_2) = -i \langle T_C [\hat{a}_{i,H}(t_1) \hat{a}_{i,H}^\dagger(t_2)] \rangle \quad (6.56)$$

This means that an equation like (5.84) attains the form

$$\begin{aligned} (i\partial_{t_1} - \mathbf{h}(t_1)) \mathbf{G}^<(t_1, t_2) &= \mathbf{\Sigma}^{\text{HF}}(t_1) \cdot \mathbf{G}^<(t_1, t_2) \\ &+ \int_{t_0}^{t_1} dt_3 [\mathbf{\Sigma}^>(t_1, t_3) - \mathbf{\Sigma}^<(t_1, t_3)] \cdot \mathbf{G}^<(t_3, t_2) - \int_{t_0}^{t_2} dt_3 \mathbf{\Sigma}^<(t_1, t_3) \cdot [\mathbf{G}^>(t_3, t_2) - \mathbf{G}^<(t_3, t_2)] \\ &- i \int_0^\beta d\tau_3 \mathbf{G}^\lceil(t_1, \tau_3) \mathbf{\Sigma}^\lceil(\tau_3, t_2) \end{aligned} \quad (6.57)$$

where all be bold-faced symbols now represent matrices and the symbol "  $\cdot$  " a matrix product. As a first application we consider a laser-excited quantum well of GaAs [14] where we only take the valence and conduction bands as basis functions. For this case the Kadanoff-Baym equations can be solved within the second Born approximation. The laser field is taken to be a 50 fs laser pulse with its maximum peak intensity at  $t = 0$ . In Figs.(6.2) and (6.3) the imaginary parts of  $G_{cc}^<$  and  $G_{vv}^<$  are displayed (both taken at the top of the valence band, i.e. in the state  $\mathbf{k} = 0$ ). As follows from Eq.(5.82) these quantities are indeed symmetric in  $t_1$  and  $t_2$ . In general one has

$$\text{Im } G_{ij}^{\lessgtr}(t_1, t_2) = \text{Im } G_{ji}^{\lessgtr}(t_2, t_1) \quad (6.58)$$

Let us see what this quantity represents. Now since

$$G_{ij}^<(t_1, t_2) = i \langle \hat{a}_{j,H}^\dagger(t_2) \hat{a}_{i,H}(t_1) \rangle \quad (6.59)$$

it follows that

$$\text{Im } G_{ii}(t_1, t_1) = \langle \hat{a}_{i,H}^\dagger(t_1) \hat{a}_{i,H}(t_1) \rangle = n_i(t_1) \quad (6.60)$$

can be interpreted as the occupation number of the state  $i$ . This is indeed consistent with figures 6.2 and 6.3. One sees that due to the laser pulse the conduction band gets occupied (the time diagonal in Fig. 6.2) whereas the valence band gets depleted (the time diagonal in Fig. 6.3). One further sees that the functions decay away from the time-diagonal. This is due to the memory terms in the Kadanoff-Baym equations, i.e. the second and the third term on the right hand side of Eq.(6.57). The decay would be absent if we would only take into account the Hartree-Fock term.

As a next application we solved the Kadanoff-Baym equations within the second Born approximation for a hydrogen molecule. The results are very recent and therefore we only plot in Fig. 6.4 the function  $\text{Im } G_{\sigma_g \sigma_g}^<(t_1, t_2)$  for a field free propagation without a laser pulse excitation. We see a similar picture as for the two-band GaAs calculations. The function oscillates away from the diagonal with a frequency that is close to the ionization energy (as it should).

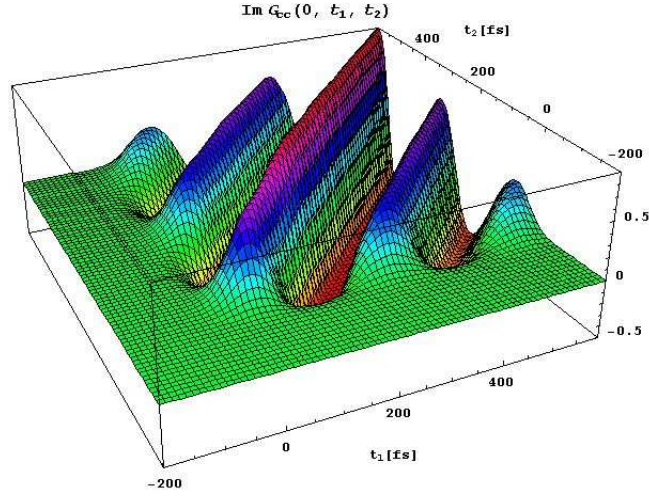


Figure 6.2: Conduction band part  $\text{Im} G_{cc}^<(t_1, t_2)$ . A  $50\text{fs}$  laser pulse is applied to GaAs which has its peak strength at  $t = 0$ . The time-diagonal gives the occupation number of the conduction band. The decay away from the time diagonal is due to electron correlations.

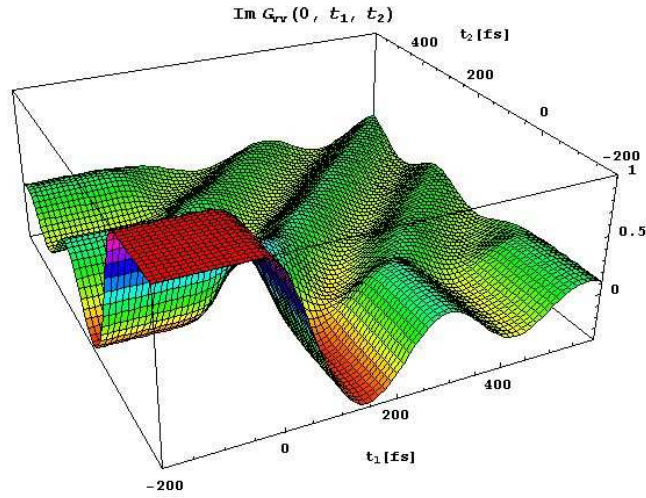


Figure 6.3: Valence band part  $\text{Im} G_{vv}^<(t_1, t_2)$ . A  $50\text{fs}$  laser pulse is applied to GaAs which has its peak strength at  $t = 0$ . The time-diagonal gives the occupation number of the valence band, it is clearly seen that the laser excitation leads to depletion of the valence band. The decay away from the time diagonal is due to electron correlations.



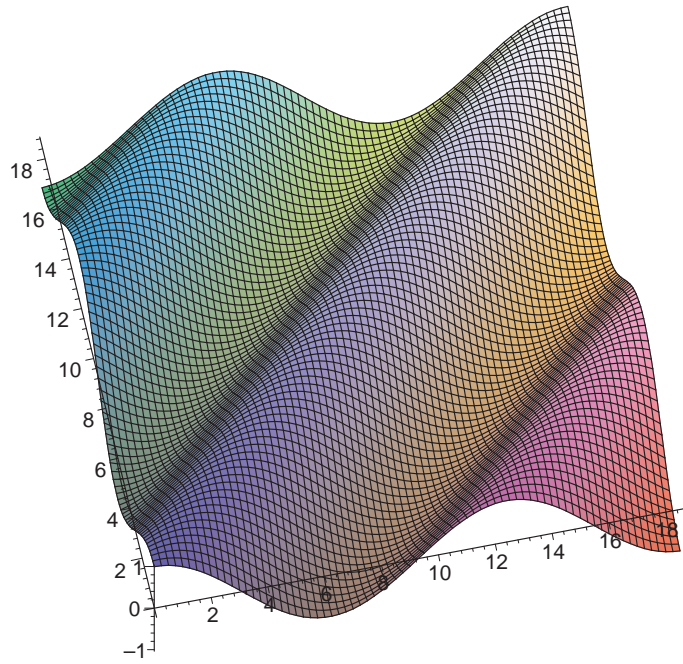


Figure 6.4:  $\text{Im} G_{\sigma_g \sigma_g}(t_1, t_2)$  for the H<sub>2</sub> molecule obtained from field free propagation of the Kadanoff-Baym equations within the second Born approximation

# Chapter 7

## The hierarchy equations

### 7.1 The Martin-Schwinger hierarchy

In this section we discuss general relations between  $n$ -particle Green functions. We start out by defining the  $n$ -body Green function as

$$\begin{aligned} G_n(1 \dots, n; 1' \dots, n') &= \frac{1}{i^n} \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) T_C \left[ \hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n') \right] \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &= (-i)^n \langle T_C [\hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \rangle \end{aligned} \quad (7.1)$$

These Green functions satisfy the following hierarchy equations

$$\begin{aligned} (i\partial_{t_1} - h(1))G_n(1, \dots, n; 1' \dots, n') &= \sum_{j=1}^n \delta(1, j') (-1)^{n-j} G_{n-1}(2 \dots, n; 1' \dots, j' - 1, j' + 1 \dots, n') \\ &\quad - i \int dx w(\mathbf{x}_1, \mathbf{x}) G_{n+1}(1 \dots, n, \mathbf{x}t_1; \mathbf{x}t_1^+, 1' \dots, n') \end{aligned} \quad (7.2)$$

This relation is a generalization of the equation of motion of the one-particle Green function and follows directly from the anti-commutation relations and the equations of motion of the field operators. The proof that we present here is therefore obtained by a straightforward albeit somewhat lengthy calculation. We first introduce a convenient notation and write

$$\begin{aligned} G_n(1 \dots, n; 1' \dots, n') &= (-i)^n \langle T_C [\hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \rangle \\ &= (-i)^n \sum_P (-1)^{\pi(P)} \theta_{2n}(t_{P(1)}, \dots, t_{P(2n)}) \langle \hat{O}_{P(1)} \dots \hat{O}_{P(2n)} \rangle \end{aligned} \quad (7.3)$$

where we renumbered  $(1' \dots, n') = (n + 1 \dots, 2n)$  and  $\pi(P)$  is the number of transpositions in the permutation  $P$ . We further defined

$$\hat{O}_i = \hat{\psi}_H(t_i) \quad \text{for } i = 1 \dots n \quad (7.4)$$

$$\hat{O}_i = \hat{\psi}_H^\dagger(t_i) \quad \text{for } i = n + 1 \dots 2n \quad (7.5)$$

We also introduced an  $n$ -time theta function

$$\theta_n(t_1, \dots, t_n) \equiv \theta(t_1, t_2)\theta(t_2, t_3) \dots \theta(t_{n-1}, t_n) \quad (7.6)$$

Then we obtain by differentiation with respect to  $t_1$  the expression

$$i\partial_{t_1} G_n(1 \dots n; 1' \dots n') = A + B \quad (7.7)$$

where

$$A = (-i)^n \sum_P i\partial_{t_1} \theta_{2n}(t_{P(1)}, \dots, t_{P(2n)}) (-1)^{\pi(P)} \langle \hat{O}_{P(1)} \dots \hat{O}_{P(2n)} \rangle \quad (7.8)$$

$$B = (-i)^n i \langle T_C[\partial_{t_1} \hat{\psi}_H(1) \hat{\psi}_H(2) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \rangle \quad (7.9)$$

Let us first concentrate on the term  $A$ . This can be written as

$$A = (-i)^{n-1} \sum_P \sum_{i=1}^{2n-1} (-1)^{\pi(P)} \theta^{(1)} \theta^{(2)} \dots \partial_{t_1} \theta^{(i)} \dots \theta^{(2n)} \langle \hat{O}_{P(1)} \dots \hat{O}_{P(2n)} \rangle \quad (7.10)$$

where we defined

$$\theta^{(i)} \equiv \theta(t_{P(i)}, t_{P(i+1)}) \quad (7.11)$$

Since

$$\partial_{t_1} \theta^{(i)} = \delta_{1, P(i)} \delta(t_1, t_{P(i+1)}) - \delta_{1, P(i+1)} \delta(t_1, t_{P(i)}) \quad (7.12)$$

Eq.(7.10) becomes

$$\begin{aligned} A &= (-i)^{n-1} \sum_{P, P(i)=1} \sum_{i=1}^{2n-1} (-1)^{\pi(P)} \delta(t_1, t_{P(i+1)}) \theta^{(1)} \dots \theta^{(i-1)} \theta^{(i+1)} \dots \theta^{(2n)} \langle \hat{O}_{P(1)} \dots \hat{O}_{P(2n)} \rangle \\ &\quad - (-i)^{n-1} \sum_{P, P(i+1)=1} \sum_{i=1}^{2n-1} (-1)^{\pi(P)} \delta(t_1, t_{P(i)}) \theta^{(1)} \dots \theta^{(i-1)} \theta^{(i+1)} \dots \theta^{(2n)} \langle \hat{O}_{P(1)} \dots \hat{O}_{P(2n)} \rangle \end{aligned} \quad (7.13)$$

Now in the second line of this equation we can write for each permutation  $P = P' \circ P_{i, i+1}$  where  $P_{i, i+1}$  is a permutation that interchanges  $i$  and  $i+1$  and replace the sum over  $P$  by a sum over  $P'$ . Since the interchange of  $i$  and  $i+1$  introduces a minus sign we obtain then for  $A$  the expression

$$\begin{aligned} A &= (-i)^{n-1} \sum_{P, P(i)=1} \sum_{i=1}^{2n-1} (-1)^{\pi(P)} \delta(t_1, t_{P(i+1)}) \theta^{(1)} \dots \theta^{(i-1)} \theta^{(i+1)} \dots \theta^{(2n)} \\ &\quad \times \langle \hat{O}_{P(1)} \dots \{ \hat{O}_{P(i)}, \hat{O}_{P(i+1)} \} \dots \hat{O}_{P(2n)} \rangle \\ &= (-i)^{n-1} \sum_{P, P(i)=1} \sum_{i=1}^{2n-1} (-1)^{\pi(P)} \delta(t_1, t_{P(i+1)}) \theta_{2n-1}(t_{P(1)}, \dots, t_{P(i-1)}, t_1, t_{P(i+2)}, \dots, t_{P(2n)}) \\ &\quad \times \{ \hat{O}_1, \hat{O}_{P(i+1)} \} \langle \hat{O}_{P(1)} \dots \hat{O}_{P(i-1)} \hat{O}_{P(i+2)} \dots \hat{O}_{P(2n)} \rangle \end{aligned} \quad (7.14)$$

Now we collect all terms with  $P(i+1) = k$  and write

$$A = (-i)^{n-1} \sum_{k=2}^{2n} \delta(t_1, t_k) \{ \hat{O}_1, \hat{O}_k \} F_k \quad (7.15)$$

where we defined

$$\begin{aligned}
F_k &= \sum_{i=1}^{2n-1} \sum_{P, P(i)=1, P(i+1)=k} (-1)^{\pi(P)} \theta_{2n-1}(t_{P(1)}, \dots, t_{P(i-1)}, t_1, t_{P(i+2)}, \dots, t_{P(2n)}) \\
&\times \langle \hat{O}_{P(1)} \dots \hat{O}_{P(i-1)} \hat{O}_{P(i+2)} \dots \hat{O}_{P(2n)} \rangle
\end{aligned} \tag{7.16}$$

This expression can be simplified if in the  $i$ -th term write the permutation  $P$  as  $P = P' \circ \bar{P}$  where  $\bar{P}$  is the permutation that maps  $(1, \dots, 2n)$  to  $(3, 4, \dots, i-1, 1, 2, i+2, \dots, 2n)$ , i.e.  $\bar{P}$  shifts the pair  $(1, 2)$  to the position  $(i, i+1)$ . We then have

$$P(i) = P'(1) = 1 \tag{7.17}$$

$$P(i+1) = P'(2) = k \tag{7.18}$$

$$P(k) = P'(k+2) \quad \text{for } k = 1, \dots, i-1 \tag{7.19}$$

$$P(k) = P'(k) \quad \text{for } k = i+1, \dots, 2n \tag{7.20}$$

We can then replace the sum over permutations by a sum over permutations  $P'$ . Since  $(-1)^{\pi(\bar{P})} = 1$  we then obtain the expression

$$\begin{aligned}
F_k &= \sum_{i=1}^{2n-1} \sum_{P, P(1)=1, P(2)=k} (-1)^{\pi(P)} \theta_{2n-1}(t_{P(3)}, \dots, t_{P(i+1)}, t_1, t_{P(i+2)}, \dots, t_{P(2n)}) \langle \hat{O}_{P(3)} \dots \hat{O}_{P(2n)} \rangle \\
&= \sum_{P, P(1)=1, P(2)=k} (-1)^{\pi(P)} \theta_{2n-2}(t_{P(3)}, \dots, t_{P(2n)}) \langle \hat{O}_{P(3)} \dots \hat{O}_{P(2n)} \rangle
\end{aligned} \tag{7.21}$$

We see that the summation over  $i$  and the dependence on  $t_1$  have disappeared from the expression. We perform a final transformation  $P' = P \circ \bar{P}$  where  $\bar{P}$  is the permutation that maps  $(1, \dots, 2n)$  to  $(1, 3, 4, \dots, k, 2, k+1, \dots, 2n)$ , i.e. it is a cyclic shift of the numbers  $(2, \dots, k)$ . Since  $(-1)^{\pi(\bar{P})} = (-1)^k$  the term  $F_k$  attains the form

$$\begin{aligned}
F_k &= (-1)^k \sum_{P', P'(1)=1, P'(k)=k} (-1)^{\pi(P')} \theta_{2n-2}(t_{P'(2)}, \dots, t_{P'(k-1)}, t_{P'(k+1)}, \dots, t_{P'(2n)}) \\
&\times \langle \hat{O}_{P'(2)} \dots \hat{O}_{P'(k-1)}, \hat{O}_{P'(k+1)}, \dots, \hat{O}_{P'(2n)} \rangle \\
&= (-1)^k \langle T_C[\hat{O}_2 \dots \hat{O}_{k-1} \hat{O}_{k+1} \dots \hat{O}_{2n}] \rangle
\end{aligned} \tag{7.22}$$

With this simple expression for  $F_k$  we can write

$$A = (-i)^{n-1} \sum_{k=2}^{2n} \delta(t_1, t_k) \left\{ \hat{O}_1, \hat{O}_k \right\} (-1)^k \langle T_C[\hat{O}_2 \dots \hat{O}_{k-1} \hat{O}_{k+1} \dots \hat{O}_{2n}] \rangle \tag{7.23}$$

If we now write the operators  $\hat{O}_k$  in terms of the field operators again we obtain the expression

$$\begin{aligned}
A &= (-i)^{n-1} \sum_{j=1}^n \delta(t_1, t'_j) \left\{ \hat{\psi}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}'_j t'_j) \right\} \\
&\times (-1)^{n+j} \langle T_C[\hat{\psi}_H(2) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger((j-1)') \hat{\psi}_H^\dagger((j+1)') \dots \hat{\psi}_H^\dagger(n')] \rangle \\
&= \sum_{j=1}^n \delta(1, j') (-1)^{n-j} G_{n-1}(2 \dots n; 1' \dots (j-1)' (j+1)' \dots n')
\end{aligned} \tag{7.24}$$

## 7.2 A simple proof of Wick's theorem

In this section we prove so-called Wick's theorem.

## 7.3 A generating functional for the $n$ -particle Green function

We now define a generating functional for the  $n$ -particle Green function. We start out by defining an extended form of the evolution operator on the time-contour as [12]:

$$\begin{aligned}\hat{U}[u](t_0 - i\beta, t_0) &= T_C \exp(-i \int d1 \hat{H}(1) - i \int d1 \int d2 \hat{\psi}^\dagger(1) u(1, 2) \hat{\psi}(2)) \\ &\equiv \hat{U}(t_0 - i\beta, t_0)[u = 0] \\ &+ \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int d1 d1' \dots dndn' T_C [\hat{\psi}_H^\dagger(1) \hat{\psi}_H(1') \dots \hat{\psi}_H^\dagger(n) \hat{\psi}_H(n')] u(1, 1') \dots u(n, n')\end{aligned}\quad (7.25)$$

In this expression  $u(1, 2)$  is function that is in general nonlocal in space and time and is only used as a convenient auxiliary quantity in the derivations and will not appear in actual applications. We will refer to it as a nonlocal potential. However, it should be pointed out that this nomenclature is somewhat misleading since it is not possible to derive a corresponding Schrödinger Hamiltonian in which this 'potential' appears, except for the case that it is local in time, i.e.  $u(1, 2) = \delta(t_1, t_2) u(\mathbf{x}_1 t_1, \mathbf{x}_2 t_1)$ . Also note that the field operators in this expression are now already given in the Heisenberg picture with respect to our many-body Hamiltonian  $\hat{H}(t)$  (which does not depend on  $u$ ). In the case  $u = 0$  this expression reduces to the evolution operator defined earlier. We now define the functional

$$Z[u] = \text{Tr} \{U(t_0 - i\beta, t_0)\} \quad (7.26)$$

Then

$$\frac{1}{Z[u]} \left. \frac{\delta Z}{\delta u(1'1)} \right|_{u=0} = -i \frac{\text{Tr} \left\{ U(t_0 - i\beta, t_0) T_C [\hat{\psi}_H^\dagger(1') \hat{\psi}_H(1)] \right\}}{\text{Tr} \{U(t_0 - i\beta, t_0)\}} = -G(1, 1') \quad (7.27)$$

We therefore have obtained the Green function as a functional derivative. More generally we can define  $n$ -body Green functions  $G_{U,n}$  which can be obtained from repeated differentiation of  $Z[u]$ , i.e.

$$\begin{aligned}\frac{1}{Z[u]} \left. \frac{\delta^n Z}{\delta u(1'1) \dots \delta u(n'n)} \right|_{u=0} &= (-i)^n \frac{\text{Tr} \left\{ U(t_0 - i\beta, t_0) T_C [\hat{\psi}_H^\dagger(1') \hat{\psi}_H(1) \dots \hat{\psi}_H^\dagger(n') \hat{\psi}_H(n)] \right\}}{\text{Tr} \{U(t_0 - i\beta, t_0)\}} \\ &= \epsilon_n (-i)^n \frac{\text{Tr} \left\{ U(t_0 - i\beta, t_0) T_C [\hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \right\}}{\text{Tr} \{U(t_0 - i\beta, t_0)\}} \\ &= \epsilon_n G_n(1 \dots n; 1' \dots n')\end{aligned}\quad (7.28)$$

where  $\epsilon_n = (-1)^{n(n+1)/2}$  and arises from reordering of the field operators. We can thus expand the functional  $Z[u]$  as a Taylor series expansion in  $u$  as

$$Z[u] = Z[0] + \sum_{n=0}^{\infty} \frac{\epsilon_n}{n!} \int d1 d1' \dots dndn' G_n(1 \dots n; 1' \dots n') u(1'1) \dots u(n'n) \quad (7.29)$$

where the term with  $n = 0$  is just defined to be one. We are now going to define  $n$ -body Green functions in the presence of the nonlocal potential  $u$  as

$$\epsilon_n G_{U,n}(1 \dots n; 1' \dots n') \equiv \frac{1}{Z[u]} \frac{\delta^n Z}{\delta u(1'1) \dots \delta u(n'n)} \quad (7.30)$$

where we do not put  $u$  is zero after differentiation. For example, one obtains for the one- and two-particle Green functions the explicit expressions

$$\begin{aligned} \frac{Z[u]}{Z[0]} G_U(11') &= G(11') \\ &- \sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \int d2d2' \dots dndn' G_n(1 \dots n; 1' \dots n') u(2'2) \dots u(n'n) \end{aligned} \quad (7.31)$$

$$\begin{aligned} \frac{Z[u]}{Z[0]} G_{U,2}(12; 1'2') &= G_2(12; 1'2') \\ &- \sum_{n=3}^{\infty} \frac{\epsilon_n}{(n-2)!} \int d3d3' \dots dndn' G_n(1 \dots n; 1' \dots n') u(3'3) \dots u(n'n) \end{aligned} \quad (7.32)$$

From these equations we can, for instance, derive an expression which will be useful later

$$\frac{\delta G(1, 1')}{\delta u(2', 2)} = G_{U,2}(12, 1'2') + G_U(1, 1') G_U(2, 2') \quad (7.33)$$

If we act with the operator  $i\partial_{t_1} - h(1)$  on both sides of Eq.(7.31) and use the Martin-Schwinger hierarchy Eq.(7.2) for the Green functions  $G_n$  and Eq.(7.32) we obtain for  $G_U$  the equation of motion

$$\begin{aligned} (i\partial_{t_1} - h(1))G_U(11') &= \delta(1 - 1') + \int d2u(12)G_U(21') \\ &- i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})G_{U,2}(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \end{aligned} \quad (7.34)$$

The derivation is straightforward but somewhat lengthy and therefore put in the Appendix. By functional differentiation with respect to  $u$  we can generate equations of motion for the higher-order Green functions. To see this we first multiply (7.34) by  $Z[u]$  to obtain

$$\begin{aligned} (i\partial_{t_1} - h_0(1))(-i)\langle 11' \rangle &= \delta(1 - 1')Z[u] + \int d\bar{1}u(1\bar{1})(-i)\langle \bar{1}1' \rangle \\ &- i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})(-i)^2 \langle 1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1' \rangle \end{aligned} \quad (7.35)$$

where we introduced the simplified notation

$$\langle 1 \dots n; 1' \dots n' \rangle = \text{Tr} \left\{ U(t_0 - i\beta, t_0) T_C [\hat{\psi}_H(1) \dots \hat{\psi}_H(n) \hat{\psi}_H^\dagger(1') \dots \hat{\psi}_H^\dagger(n')] \right\} \quad (7.36)$$

We use the convention that the primed variables are always associated with creation operators and that the unprimed variables are always associated with the annihilation operators. Taking the functional derivative of Eq.(7.35) with respect to  $u(2'2)$  then gives

$$\begin{aligned} (i\partial_{t_1} - h_0(1))(-i)^2 \langle 11'2'2 \rangle &= \delta(1 - 1')(-i)\langle 2'2 \rangle + \delta(1 - 2')(-i)\langle 21' \rangle \\ &+ \int d\bar{1}u(1\bar{1})(-i)^2 \langle \bar{1}1'2'2 \rangle - i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})(-i)^3 \langle 1, \mathbf{x}t_1, \mathbf{x}t_1^+, 1'2'2 \rangle \end{aligned} \quad (7.37)$$

Reordering the indices and dividing by  $Z[u]$  then gives

$$\begin{aligned}
& (i\partial_{t_1} - h_0(1))G_{2,U}(12; 1'2') = -\delta(1 - 1')G_U(22') + \delta(1 - 2')G_U(21') \\
& + \int d\bar{1}u(1\bar{1})G_{2,U}(\bar{1}2; 1'2') - i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})G_{3,U}(12, \mathbf{x}t_1; \mathbf{x}t_1^+, 1'2')
\end{aligned} \tag{7.38}$$

This is the second equation of the Martin-Schwinger hierarchy. By continued differentiation we obtain the general hierarchy equations for  $G_{n,U}$

$$\begin{aligned}
& (i\partial_{t_1} - h_0(1))G_{n,U}(1, \dots, n; 1' \dots n') \\
& = \sum_{j=1}^n \delta(1, j')(-1)^{n-j}G_{n-1,U}(2 \dots n; 1' \dots j' - 1, j' + 1 \dots n') \\
& + \int d\bar{1}u(1, \bar{1})G_{n,U}(\bar{1}2 \dots n; 1' \dots n') - i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})G_{n+1,U}(1 \dots n, \mathbf{x}t_1; \mathbf{x}t_1^+, 1' \dots n')
\end{aligned} \tag{7.39}$$

These equations are readily proven by induction if we multiply them by  $Z[u]$  and take the functional derivative with respect to  $u(n' + 1, n + 1)$ . Finally we remark on the boundary conditions. From Eqs.(7.31) and (7.32) we see that  $G_U$  and  $G_{U,2}$  also satisfy the Kubo-Martin-Schwinger conditions in case they are satisfied by the Green functions  $G_n$ .

# Chapter 8

## General initial states

### 8.1 Structure of the self-energy

Instead of starting from an equilibrium situation we will now discuss the propagation of the Green function from a general initial ensemble  $\hat{\rho}$ . The Green function is then defined as

$$G(1, 2) = -i\langle\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\rangle \equiv -i \text{Tr} \left\{ \hat{\rho} \hat{\psi}_H(1)\hat{\psi}_H^\dagger(2) \right\} \quad (8.1)$$

In a similar manner we can also define the  $n$ -particle Green functions. The choice of the initial conditions for the time-propagation must now reflect the choice of the initial density matrix. The special case

$$\hat{\rho} = |\Psi_0\rangle\langle\Psi_0| \quad (8.2)$$

where  $|\Psi_0\rangle$  is the ground state of the system is then related to the zero-temperature limit of the formalism discussed earlier. The main feature of the present formalism that we now no longer have to deal with the imaginary part of the contour which was responsible for the initial conditions. The contour now simply goes from  $t_0$  back and forth on the real axis. However, nothing changes in the derivation of the equations of motion which only depend on the anti-commutation relations and the form of the Hamiltonian.

We start with the equations of motion of the Green function:

$$(i\partial_{t_1} - h(1))G(1, 1') = \delta(1, 1') - i \int d2 w(1^+, 2)G_2(1, 2, 2^+, 1') \quad (8.3)$$

$$(-i\partial_{t'_1} - h(1'))G(1, 1') = \delta(1, 1') - i \int d2 w(1'^+, 2)G_2(1, 2, 2^+, 1') \quad (8.4)$$

and define the self-energy and its adjoint by the equations

$$\begin{aligned} \int d\bar{1} \Sigma(1, \bar{1})G(\bar{1}, 1') &= -i \int d2 w(1^+, 2)G_2(1, 2, 2^+, 1') \\ &= -i\langle T_C[\hat{i}_H(1)\hat{\psi}^\dagger(1')] \rangle \end{aligned} \quad (8.5)$$

$$\begin{aligned} \int d\bar{1} G(1, \bar{1})\hat{\Sigma}(\bar{1}, 1') &= -i \int d2 w(1'^+, 2)G_2(1, 2, 2^+, 1') \\ &= -i\langle T_C[\hat{\psi}_H(1)\hat{i}_H^\dagger(1')] \rangle \end{aligned} \quad (8.6)$$



where we defined the operators

$$\hat{i}_H(1) = \int d2 w(1,2) \hat{\psi}_H^\dagger(2) \hat{\psi}_H(2) \hat{\psi}_H(1) \quad (8.7)$$

$$\hat{i}_H^\dagger(1) = \int d2 w(1,2) \hat{\psi}_H^\dagger(1) \hat{\psi}_H^\dagger(2) \hat{\psi}_H(2) \quad (8.8)$$

which are each others adjoints. These operators appear directly form the equation of motion of the field operators

$$(i\partial_{t_1} - h(1))\hat{\psi}_H(1) = \hat{i}_H(1) \quad (8.9)$$

$$(-i\partial_{t_1} - h(1))\hat{\psi}_H^\dagger(1) = \hat{i}_H^\dagger(1) \quad (8.10)$$

In the case of general initial states we can not rely on the Kubo-Martin-Schwinger conditions to specify the initial conditions. The main question now how to specify the initial conditions and how it affects the self-energy. The equations of motion must be solved by specifying an initial one-particle density-matrix  $\gamma$

$$G^<(\mathbf{x}_1 t_0, \mathbf{x}_2 t_0) = i\langle \hat{\psi}_H^\dagger(\mathbf{x}_2, t_0) \hat{\psi}_H(\mathbf{x}_1 t_0) \rangle = i\gamma(\mathbf{x}_2, \mathbf{x}_1, t_0) \quad (8.11)$$

However, apart from a one-particle Green function the equations of motion also contain a 2-particle Green function. This means that the self-energy also must depend on an initial 2-particle Green function, i.e. on an initial 2-particle density matrix. This can be seen by considering the limits

$$\lim_{t_1, t'_1 \rightarrow t_0} \int d\bar{1} \Sigma(1, \bar{1}) G(\bar{1}, 1') = \lim_{t_1, t'_1 \rightarrow t_0} -i\langle T_C [\hat{i}_H(1) \hat{\psi}^\dagger(1')] \rangle \quad (8.12)$$

$$\lim_{t_1, t'_1 \rightarrow t_0} \int d\bar{1} G(1, \bar{1}) \hat{\Sigma}(\bar{1}, 1') = \lim_{t_1, t'_1 \rightarrow t_0} -i\langle T_C [\hat{\psi}_H(1) \hat{i}_H^\dagger(1')] \rangle \quad (8.13)$$

The right hand sides of these equations do not go to zero. However, the lenght ( which runs to the maximum value of  $t_1$  and  $t'_1$ ) can be taken increasingly smaller. Therefore to obtain a finite answer after the contour integration the selfenergies  $\Sigma$  and  $\hat{\Sigma}$  must contain delta-function-like singularities. One such singular term is simply the Hartree-Fock time term  $\Sigma^\delta(1, 1') \sim \delta(t_1, t'_1)$ . However, if this were the only term then from the equations (8.12) and (8.13) we would have that initial two-particle Green function would simply be an uncorrelated product of one-particle Green functions. Therefore, in general there must be another singular part in the Green function which must correspond to a delta function situated at  $t_0$ . The selfenergies therefore have the form

$$\Sigma(1, 1') = \Sigma_{\text{in}}(1, 1') + \bar{\Sigma}(1, 1') \quad (8.14)$$

$$\hat{\Sigma}(1, 1') = \hat{\Sigma}_{\text{in}}(1, 1') + \hat{\bar{\Sigma}}(1, 1') \quad (8.15)$$

The terms  $\bar{\Sigma}$  and  $\hat{\bar{\Sigma}}$  denote the parts of the self-energy that are not singular at  $t_0$ . The self-energies  $\Sigma_{\text{in}}$  and  $\hat{\Sigma}_{\text{in}}$  which describe the initial correlations are of the form

$$\Sigma_{\text{in}}(1, 1') = f_-(1, \mathbf{x}'_1 t_0) \delta(t'_1, t_0^-) + f_+(1, \mathbf{x}'_1 t_0) \delta(t'_1, t_0^+) \quad (8.16)$$

$$\hat{\Sigma}_{\text{in}}(1, 1') = \hat{f}_-(\mathbf{x}_1 t_0, 1') \delta(t_1, t_0^-) + \hat{f}_+(\mathbf{x}_1 t_0, 1') \delta(t_1, t_0^+) \quad (8.17)$$

The times  $t_0^-$  and  $t_0^+$  are the contour variables at the beginning and the end of the contour and  $\delta(t, t_0^\pm)$  are the corresponding contour delta functions. This means that if we parametrize the contour  $t(s)$  by an underlying parameter running from  $s_-$  to  $s_+$  with  $t(s_-) = t(s_+) = t_0$  then

$\delta(t, t_0^\pm) = \delta(s - s_\pm)/(dt/ds)(s_\pm)$ . The functions  $f_\pm$  and  $\hat{f}_\pm$  are functions to be determined. We will show that  $f_+ = -f_-$  and  $\hat{f}_+ = -\hat{f}_-$ . However we will start out by proving that for the noninitial parts of the selfenergy we have  $\bar{\Sigma} = \hat{\Sigma}$ . We start by calculating

$$\begin{aligned} \int d2 \Sigma_{\text{in}}(1, 2)G(2, 1') &= \int d\mathbf{x}_2 f_+(1, \mathbf{x}_2 t_0)G^>(\mathbf{x}_2 t_0, 1') + f_-(1, \mathbf{x}_2 t_0)G^<(\mathbf{x}_2 t_0, 1') \\ &= -i \int d\mathbf{x}_2 f_+(1, \mathbf{x}_2 t_0)\langle \hat{\psi}_H(\mathbf{x}_2 t_0)\hat{\psi}_H^\dagger(1') \rangle + i \int d\mathbf{x}_2 f_-(1, \mathbf{x}_2 t_0)\langle \hat{\psi}_H^\dagger(1')\hat{\psi}_H(\mathbf{x}_2 t_0) \rangle \end{aligned} \quad (8.18)$$

$$\begin{aligned} \int d2 G(1, 2)\hat{\Sigma}_{\text{in}}(2, 1') &= \int d\mathbf{x}_2 G^<(1, \mathbf{x}_2 t_0)f_+(\mathbf{x}_2 t_0, 1') + G^>(1, \mathbf{x}_2 t_0)f_-(\mathbf{x}_2 t_0, 1') \\ &= i \int d\mathbf{x}_2 \langle \hat{\psi}_H^\dagger(\mathbf{x}_2 t_0)\hat{\psi}_H(1) \rangle f_+(\mathbf{x}_2 t_0) - i \int d\mathbf{x}_2 \langle \hat{\psi}_H(1)\hat{\psi}_H^\dagger(\mathbf{x}_2 t_0) \rangle f_-(\mathbf{x}_2 t_0) \end{aligned} \quad (8.19)$$

From these expression we now calculate using Eqs.(8.9) and (8.10)

$$\begin{aligned} (-i\partial_{t'_1} - h(1')) \int_C d2 \Sigma_{\text{in}}(1, 2)G(2, 1') \\ &= -i \int d\mathbf{x}_2 f_+(1, \mathbf{x}_2 t_0)\langle \hat{\psi}_H(\mathbf{x}_2 t_0)\hat{i}_H^\dagger(1') \rangle + i \int d\mathbf{x}_2 f_-(1, \mathbf{x}_2 t_0)\langle \hat{i}_H^\dagger(1')\hat{\psi}_H(\mathbf{x}_2 t_0) \rangle \\ &= -i \int d2 \Sigma_{\text{in}}(1, 2)\langle T_C[\hat{\psi}_H(2)\hat{i}_H^\dagger(1')] \rangle = \int d2d3 \Sigma_{\text{in}}(1, 2)G(2, 3)\hat{\Sigma}(3, 1') \end{aligned} \quad (8.20)$$

and similarly

$$\begin{aligned} (i\partial_{t_1} - h(1)) \int d2 G(1, 2)\hat{\Sigma}_{\text{in}}(2, 1') \\ &= i \int d\mathbf{x}_2 \langle \hat{\psi}_H^\dagger(\mathbf{x}_2 t_0)\hat{i}_H(1) \rangle f_+(\mathbf{x}_2 t_0) - i \int d\mathbf{x}_2 \langle \hat{i}_H(1)\hat{\psi}_H^\dagger(\mathbf{x}_2 t_0) \rangle f_-(\mathbf{x}_2 t_0) \\ &= -i \int d2 \langle T_C[\hat{i}_H(1)\hat{\psi}_H^\dagger(2)] \rangle \hat{\Sigma}_{\text{in}}(2, 1') = \int d2d3 \Sigma(1, 3)G(3, 2)\hat{\Sigma}_{\text{in}}(2, 1') \end{aligned} \quad (8.21)$$

Note that in the derivations we have not assumed anything about the specific form of  $f_\pm$ . So for any function  $A(1, 1')$  and  $\hat{A}(1, 1')$  of the form

$$A(1, 1') = a_-(1, \mathbf{x}'_1 t_0) \delta(t'_1, t_0^-) + a_+(1, \mathbf{x}'_1 t_0) \delta(t'_1, t_0^+) \quad (8.22)$$

$$\hat{A}(1, 1') = \hat{a}_-(\mathbf{x}_1 t_0, 1') \delta(t_1, t_0^-) + \hat{a}_+(\mathbf{x}_1 t_0, 1') \delta(t_1, t_0^+) \quad (8.23)$$

we have

$$(i\partial_{t_1} - h(1)) \int d2 G(1, 2)A(2, 1') - \int d2d3 \Sigma(1, 3)G(3, 2)A(2, 1') = 0 \quad (8.24)$$

$$(-\partial_{t'_1} - h(1')) \int d2 \hat{A}(1, 2)G(2, 1') - \int d2d3 \hat{A}(1, 3)G(3, 2)\hat{\Sigma}(2, 1') = 0 \quad (8.25)$$

Note that it would have been tempting to use in Eqs.(8.20) and Eq.(8.21) directly the equations of motion

$$(i\partial_{t_1} - h(1))G(1, 2) = \delta(1, 2) + \int d3 \Sigma(1, 3)G(3, 2) \quad (8.26)$$

$$(-i\partial_{t'_1} - h(1'))G(2, 1') = \delta(2, 1') + \int d3 G(1, 3)\hat{\Sigma}(3, 1') \quad (8.27)$$

Then, for instance in Eq.(8.21), we would have had to give mathematical meaning to expressions of the form  $\delta(t_2, t_0^\pm)\delta(t_2, t_1')$ . However, since the delta function  $\delta(t_2, t_1')$  arises from differentiation of the contour ordering theta-function  $\theta(t_2, t_1')$  in the definition of the Green function, it has only mathematical meaning for  $t_0^- < t_1', t_2 < t_0^+$  on the contour. For this reason we proceeded more carefully and first integrated out the initial time delta functions before differentiation in Eqs.(8.20) and (8.21). We can use the equations of motion directly, however, for the noninitial parts of the self-energy, which were defined in Eqs.(8.14) and (8.15). For these quantities we have

$$(-i\partial_{t_1'} - h(1')) \int d2 \bar{\Sigma}(1, 2)G(2, 1') = \bar{\Sigma}(1, 1') + \int d2d3 \bar{\Sigma}(1, 2)G(2, 3)\hat{\Sigma}(3, 1') \quad (8.28)$$

$$(i\partial_{t_1} - h(1)) \int d2 G(1, 2)\hat{\Sigma}(2, 1') = \hat{\Sigma}(1, 1') + \int d2d3 \Sigma(1, 2)G(2, 3)\hat{\Sigma}(3, 1') \quad (8.29)$$

Together with Eqs.(8.20) and (8.21) we therefore obtain

$$(-i\partial_{t_1'} - h(1')) \int d2 \Sigma(1, 2)G(2, 1') = \bar{\Sigma}(1, 1') + \int d2d3 \Sigma(1, 2)G(2, 3)\hat{\Sigma}(3, 1') \quad (8.30)$$

$$(i\partial_{t_1} - h(1)) \int d2 G(1, 2)\hat{\Sigma}(2, 1') = \hat{\Sigma}(1, 1') + \int d2d3 \Sigma(1, 2)G(2, 3)\hat{\Sigma}(3, 1') \quad (8.31)$$

From Eq.(8.5) and (8.6) on the other hand we have

$$(-i\partial_{t_1'} - h(1')) \int d2 \bar{\Sigma}(1, 2)G(2, 1') = i\delta(t_1, t_1')\langle\{\hat{i}_H(1), \hat{\psi}_H^\dagger(1')\}\rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(1')]\rangle \quad (8.32)$$

$$(i\partial_{t_1} - h(1)) \int d2 G(1, 2)\hat{\Sigma}(2, 1') = i\delta(t_1, t_1')\langle\{\hat{\psi}_H(1), \hat{i}_H^\dagger(1')\}\rangle - i\langle T_C[\hat{i}_H(1)\hat{i}_H^\dagger(1')]\rangle \quad (8.33)$$

As was done in Chapter 5, one can readily check using the equal time commutation relations of the field operators that the equal time parts on the right hand sides of Eqs.(8.32) and (8.33) are equal

$$\langle\{\hat{i}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}'_1 t_1)\}\rangle = \langle\{\hat{\psi}_H(\mathbf{x}_1 t_1), \hat{i}_H^\dagger(\mathbf{x}'_1 t_1)\}\rangle \quad (8.34)$$

and therefore Eqs.(8.32) and (8.33) together with Eqs.(8.30) and (8.31) imply that

$$\bar{\Sigma}(1, 1') = \hat{\Sigma}(1, 1') \quad (8.35)$$

Therefore the noninitial part of the selfenergy and the noninitial part of the adjoint selfenergy are the same. In other words

$$\Sigma(1, 1') = \hat{\Sigma}(1, 1') \quad \text{if } t_1, t_1' \neq t_0 \quad (8.36)$$

We also see from our derivations that the self-energy has the structure

$$\Sigma(1, 1') = \Sigma_{\text{in}}(1, 1') + \Sigma^\delta(1, 1') + \theta(t_1, t_1')\Sigma^>(1, 1') + \theta(t_1', t_1)\Sigma^<(1, 1') \quad (8.37)$$

$$\hat{\Sigma}(1, 1') = \hat{\Sigma}_{\text{in}}(1, 1') + \Sigma^\delta(1, 1') + \theta(t_1, t_1')\Sigma^>(1, 1') + \theta(t_1', t_1)\Sigma^<(1, 1') \quad (8.38)$$

where

$$\Sigma^\delta(1, 1') = \delta(t_1, t_1')\langle\{\hat{i}_H(\mathbf{x}_1 t_1), \hat{\psi}_H^\dagger(\mathbf{x}'_1 t_1)\}\rangle \quad (8.39)$$

Our next task is to derive self-consistent equations that express the self-energy in terms of the Green functions. This will be the topic of the next section.

## 8.2 Derivation of self-consistent equations

For our derivations it is convenient to work with the equations of motion of the Martin-Schwinger hierarchy in the presence of the nonlocal potential  $u$ :

$$\begin{aligned} (i\partial_{t_1} - h(1))G_U(1, 1') &= \delta(1, 1') + \int d\bar{1} u(1, \bar{1})G_U(\bar{1}, 1') - i \int d\mathbf{x} w(\mathbf{x}_1, \mathbf{x})G_{U,2}(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \\ &= \delta(1, 1') + \int d\bar{1} u(1, \bar{1})G_U(\bar{1}, 1') + \int d2 \Sigma(1, \bar{1})G_U(\bar{1}, 1') \end{aligned} \quad (8.40)$$

$$\begin{aligned} (-i\partial_{t'_1} - h(1'))G_U(1, 1') &= \delta(1, 1') + \int d\bar{1} G_U(1, \bar{1})u(\bar{1}, 1') - i \int d\mathbf{x} w(\mathbf{x}'_1, \mathbf{x})G_{U,2}(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \\ &= \delta(1, 1') + \int d2 G_U(1, \bar{1})u(\bar{1}, 1') + \int d\bar{1} G(1, \bar{1})\hat{\Sigma}(\bar{1}, 1') \end{aligned} \quad (8.41)$$

For notational convenience, however, we will drop the subindex  $U$  and will in the following always assume the Green functions to be functionals of  $u$ . If we differentiate Eq.(8.40) and (8.41) with respect to  $u(2', 2)$  we obtain the equations

$$\begin{aligned} (i\partial_{t_1} - h(1))\frac{\delta G(1, 1')}{\delta u(2', 2)} &- \int d\bar{1} (u(1, \bar{1}) + \Sigma(1, \bar{1}))\frac{\delta G(\bar{1}, 1')}{\delta u(2', 2)} \\ &= \delta(1, 2')G(2, 1') + \int d\bar{1} \frac{\delta \Sigma(1, \bar{1})}{\delta u(2', 2)}G(\bar{1}, 1') \end{aligned} \quad (8.42)$$

$$\begin{aligned} (-i\partial_{t'_1} - h(1'))\frac{\delta G(1, 1')}{\delta u(2', 2)} &- \int d\bar{1} \frac{\delta G(1, \bar{1})}{\delta u(2', 2)}(u(\bar{1}, 1') + \hat{\Sigma}(\bar{1}, 1')) \\ &= G(1, 2')\delta(2, 1') + \int d\bar{1} G(1, \bar{1})\frac{\delta \hat{\Sigma}(\bar{1}, 1')}{\delta u(2', 2)} \end{aligned} \quad (8.43)$$

$$(8.44)$$

The general solution to these two equations is given by

$$\begin{aligned} \frac{\delta G(1, 1')}{\delta u(2', 2)} &= G(1, 2')G(2, 1') \\ &+ \int d\bar{1} d\bar{1}' G(1, \bar{1}) \frac{\delta(\bar{\Sigma}(\bar{1}, \bar{1}') + \Sigma_{\text{in}}(\bar{1}, \bar{1}') + \hat{\Sigma}_{\text{in}}(\bar{1}, \bar{1}'))}{\delta u(2', 2)} G(\bar{1}, 1') + C(1, 2, 1', 2') \end{aligned} \quad (8.45)$$

where the function  $C(1, 2, 1', 2')$  satisfies

$$(i\partial_{t_1} - h(1))C(1, 2, 1', 2') - \int d\bar{1} (u(1, \bar{1}) + \Sigma(1, \bar{1}))C(\bar{1}, 2, 1', 2') = 0 \quad (8.46)$$

$$(-i\partial_{t'_1} - h(1'))C(1, 2, 1', 2') - \int d\bar{1} C(1, 2, \bar{1}, 2')(u(\bar{1}, 1') + \hat{\Sigma}(\bar{1}, 1')) = 0 \quad (8.47)$$

The Eq.(8.45) is readily proven using the equations of motion of the Green function and the observation that the terms  $\delta \Sigma_{\text{in}}/\delta u$  and  $\delta \hat{\Sigma}_{\text{in}}/\delta u$  are of the form of Eqs.(8.22) and (8.23) and therefore satisfy Eq.(8.24) and (8.25). We further know (see Eq.(7.33)) that

$$\frac{\delta G(1, 1')}{\delta u(2', 2)} = G_2(1, 2, 1', 2') + G(1, 1')G(2, 2') \quad (8.48)$$

We can therefore rewrite Eq.(8.45) as

$$\begin{aligned}
G_2(1, 2, 1', 2') &= G(1, 2')G(2, 1') - G(1, 1')G(2, 2') + C(1, 2, 1', 2') \\
&+ \int d\bar{1}d\bar{1}'G(1, \bar{1})\frac{\delta(\bar{\Sigma}(\bar{1}, \bar{1}') + \Sigma_{\text{in}}(\bar{1}, \bar{1}') + \hat{\Sigma}_{\text{in}}(\bar{1}, \bar{1}'))}{\delta u(2', 2)}G(\bar{1}, 1')
\end{aligned} \tag{8.49}$$

Now we can safely assume that  $C$  has the same symmetries as the two-particle Green function  $G_2$ , i.e.

$$C(1, 2, 1', 2') = -C(2, 1, 1', 2') = -C(1, 2, 2', 1') = C(2, 1, 2', 1') \tag{8.50}$$

Therefore in addition to (8.46) and (8.47) the function  $C$  satisfies

$$(i\partial_{t_2} - h(2))C(1, 2, 1', 2') - \int d\bar{1}(u(2, \bar{1}) + \Sigma(2, \bar{1}))C(1, \bar{1}, 1', 2') = 0 \tag{8.51}$$

$$(-i\partial_{t'_2} - h(2'))C(1, 2, 1', 2') - \int d\bar{1}C(1, 2, 1, \bar{1})(u(\bar{1}, 2') + \hat{\Sigma}(\bar{1}, 2')) = 0 \tag{8.52}$$

We thus have a complete set of four equations for the function  $C$ . We still have to determine the initial value. From Eq.(8.49) we see that

$$\lim_{t_1, t'_1 \rightarrow t_0} C(1, 2, 1', 2') = \lim_{t_1, t'_1 \rightarrow t_0} [G_2(1, 2, 1', 2') - G(1, 2')G(2, 1') + G(1, 1')G(2, 2')] \tag{8.53}$$

since in this limit the last term in Eq.(8.49) with the contour integral vanishes. Let us therefore study the limit

$$C(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}'_1, \mathbf{x}'_2) = \lim_{t_1, t'_1, t_2, t'_2 \rightarrow t_0} C(1, 2, 1', 2') \tag{8.54}$$

This limit is, as we will see, independent on the order in which the different time limits are taken.

### 8.3 Kadanoff-Baym equations for general initial states

## Chapter 9

# Outlook

In these notes we have given an introduction to the nonequilibrium Green function method, starting from basic ideas based on the time contour to the final derivation of the Kadanoff-Baym equations which are the ones that need to be solved in practical applications. Due to the limited space necessarily many things have been left out. Many things can still be said about the properties of the spectral functions that can be calculated from the nonequilibrium Green function method and which are related to other exact identities known as the Ward identities. Also the topic of more general initial states than the equilibrium state has been left out. The properties of the  $\Phi$ -functional have only been briefly touched and other conserving schemes such as the GW-method and the T-matrix approximation have not been discussed at all.

Nevertheless we believe that the background presented here will provide the reader with enough information to study the wide literature on transport through single molecules, as well as many other applications of nonequilibrium Green function theory. Especially with the developments in single molecule conduction the interest in the nonequilibrium Green function method has been growing steadily and is likely to do so in the near future.

## Appendix A

# The Martin-Schwinger hierarchy with nonlocal external potentials

We will now derive the equation of motion of  $G_U$ . If we act with  $i\partial_{t_1} - h_0(1)$  on both sides of Eq.(7.31) we obtain

$$\begin{aligned} \frac{Z[u]}{Z[0]}(i\partial_{t_1} - h_0(1))G_U(11') &= \delta(1 - 1') - i \int d\mathbf{x} w(\mathbf{x}_1, \mathbf{x}) G_2(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \\ &- \sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \int d2d2' \dots dndn' (i\partial_{t_1} - h_0(1))G_n(1 \dots n; 1' \dots n') u(2'2) \dots u(n'n) \end{aligned} \quad (\text{A.1})$$

If we use the equations of motion of  $G_n$  we can write this as

$$\begin{aligned} \frac{Z[u]}{Z[0]}(i\partial_{t_1} - h_0(1))G_U(11') &= \delta(1 - 1') - i \int d\mathbf{x} w(\mathbf{x}_1, \mathbf{x}) G_2(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \\ &+ \delta(1 - 1')A + B + C \end{aligned} \quad (\text{A.2})$$

where

$$\begin{aligned} A &= - \sum_{n=2}^{\infty} \frac{\epsilon_n (-1)^{n-1}}{(n-1)!} \int d2d2' \dots dndn' G_{n-1}(2 \dots n; 2' \dots n') u(2'2) \dots u(n'n) \\ B &= - \sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \int d2d2' \dots dndn' \sum_{j=2}^n \delta(1 - j') (-1)^{n-j} G_{n-1}(2 \dots n; 1' \dots j' - 1, j' + 1 \dots n') \\ &\times u(2'2) \dots u(n'n) \\ C &= i \int d\mathbf{x} w(\mathbf{x}_1, \mathbf{x}) \sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \int d2d2' \dots dndn' G_{n+1}(1 \dots n, \mathbf{x}t_1; \mathbf{x}t_1^+, 1'2' \dots n') \end{aligned} \quad (\text{A.3})$$

Now  $A$  can be simply rewritten to give

$$\begin{aligned} A &= - \sum_{n=1}^{\infty} \frac{\epsilon_{n+1} (-1)^n}{n!} \int d1d1' \dots dndn' G_n(1 \dots n; 1' \dots n') u(1'1) \dots u(n'n) \\ &= \sum_{n=1}^{\infty} \frac{\epsilon_n}{n!} \int d1d1' \dots dndn' G_n(1 \dots n; 1' \dots n') u(1'1) \dots u(n'n) = \frac{Z[u]}{Z[0]} - 1 \end{aligned} \quad (\text{A.4})$$

where we used that  $\epsilon_{n+1}(-1)^n = -\epsilon_n$ . The term  $B$  can be rewritten as

$$\begin{aligned}
B &= -\sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \sum_{j=2}^n \int dj u(1, j) \int d2d2' \dots \widehat{dj} \widehat{dj'} \dots dndn' (-1)^{n-j} G_{n-1}(2 \dots n; 1' \dots \widehat{j'} \dots n') \\
&\times u(2'2) \dots \widehat{u(j'j)} \dots u(n'n) \\
&= \int d2u(1, 2)G(2, 1') \\
&- \sum_{n=3}^{\infty} \frac{\epsilon_n}{(n-1)!} \sum_{j=2}^n \int dj u(1, j) \int d2d2' \dots \widehat{dj} \widehat{dj'} \dots dndn' (-1)^{n-j} G_{n-1}(2 \dots n; 1' \dots \widehat{j'} \dots n') \\
&\times u(2'2) \dots \widehat{u(j'j)} \dots u(n'n) \tag{A.5}
\end{aligned}$$

where we extracted the term with  $n = 2$  and where the  $\widehat{j}$  denotes the fact that this variable is left out. We now use

$$G_{n-1}(2 \dots n; 1' \dots \widehat{j'} \dots n') = (-1)^{j-2} G_{n-1}(j, 2 \dots \widehat{j} \dots n; 1' \dots \widehat{j'} \dots n') \tag{A.6}$$

With this relation we see that after the summation sign over  $j$  we obtain  $(n-1)$  identical terms. If we take the term with  $j = n$  and relabel  $j = \bar{1}$  and the remaining integration variables as  $2 \dots n-1, 2' \dots n'-1$  we obtain

$$\begin{aligned}
B &- \int d\bar{1}u(1, \bar{1})G(\bar{1}, 1') = \\
&- \sum_{n=3}^{\infty} \frac{\epsilon_n (-1)^{n-2}}{(n-2)!} \int d\bar{1} u(1, \bar{1}) \int d2d2' \dots d(n-1)d(n'-1) G_{n-1}(\bar{1}2 \dots n-1; 1' \dots n'-1) \\
&\times u(2'2) \dots u(n'-1, n-1) \\
&= -\sum_{n=2}^{\infty} \frac{\epsilon_{n+1} (-1)^{n-1}}{(n-1)!} \int d\bar{1} u(1, \bar{1}) \int d2d2' \dots dndn' G_n(\bar{1}2 \dots n; 1' \dots n') u(2'2) \dots u(n', n) \\
&= -\sum_{n=2}^{\infty} \frac{\epsilon_n}{(n-1)!} \int d\bar{1} u(1, \bar{1}) \int d2d2' \dots dndn' G_n(\bar{1}2 \dots n; 1' \dots n') u(2'2) \dots u(n', n) \\
&= \int d\bar{1}u(1, \bar{1}) \left[ \frac{Z[u]}{Z[0]} G_U(\bar{1}, 1) - G(\bar{1}, 1) \right] \tag{A.7}
\end{aligned}$$

where we used that  $\epsilon_{n+1}(-1)^{n-1} = \epsilon_n$ . We therefore obtain

$$B = \frac{Z[u]}{Z[0]} \int d\bar{1}u(1, \bar{1})G_U(\bar{1}, 1) \tag{A.8}$$

This leaves us with term  $C$ . This can be rewritten as

$$\begin{aligned}
C &= i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x}) \sum_{n=3}^{\infty} \frac{\epsilon_{n-1}}{(n-2)!} \int d3d3' \dots dndn' G_n(1, 3 \dots n, \mathbf{x}t_1; \mathbf{x}t_1^+, 1'3' \dots n') \\
&= i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x}) \sum_{n=3}^{\infty} \frac{\epsilon_{n-1}(-1)^{n-2}}{(n-2)!} \int d3d3' \dots dndn' G_n(1, \mathbf{x}t_1, 3 \dots n; \mathbf{x}t_1^+, 1'3' \dots n') \\
&= i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x}) \sum_{n=3}^{\infty} \frac{\epsilon_n}{(n-2)!} \int d3d3' \dots dndn' G_n(1, \mathbf{x}t_1, 3 \dots n; \mathbf{x}t_1^+, 1'3' \dots n') \\
&= -i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x}) \left[ \frac{Z[u]}{Z[0]} G_{2,U}(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') - G_2(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1') \right] \tag{A.9}
\end{aligned}$$



Collecting our results we finally obtain

$$\begin{aligned}
(i\partial_{t_1} - h_0(1))G_U(11') &= \delta(1 - 1') + \int d\bar{1}u(\bar{1}\bar{1})G_U(\bar{1}\bar{1}') \\
&- i \int d\mathbf{x}w(\mathbf{x}_1, \mathbf{x})G_{U,2}(1, \mathbf{x}t_1; \mathbf{x}t_1^+, 1')
\end{aligned} \tag{A.10}$$

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