

Study of linear response in Hubbard chains using Many-body Perturbation Theory

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Master's thesis
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Abstract

In this work the basic formalism of non-equilibrium Green's functions is presented and then applied to study a Ward identity in linear response theory, namely the frequency sum-rule. It can be proven that the frequency sum-rule is satisfied when the quantities involved are calculated using perturbation theory within a conserving approximation for the self-energy. To illustrate this equality along with other properties of the response function, a numerical application that solves the Kadanoff-Baym equations for systems of Hubbard chains was used. The results showed that the frequency sum-rule was satisfied to the same extent by all the conserving approximations used as by the exact diagonalization numerical results. The density response function was analyzed diagrammatically for a series of conserving approximations for the self-energy and this demonstrated that even for a first order in perturbation theory approximation for Σ , the response function has a corresponding complex, third order in the perturbation diagrammatic structure.

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Introduction

Nanoscience studies and manipulates chemical and biological structures of sizes between that of a few atoms to hundreds of nanometers. Its purpose is to control the functionality of matter and its assembly at the nanometer length scale and engineer devices out of molecular or biological entities that can exchange information with the macroscopic world.

This vision can be approached from two directions. One is the "top-down" paradigm which aims at reducing the size of machines designed in the macroscopic world until they fit into the microscopic one. The other approach is called "bottom-up" and tries to assemble devices inside the microscopic world starting from atoms and building its way up to more complex structures.

For the latter, it is important to study systems of atoms and molecules. To solve such systems, in principle it is only necessary to find the solution of the Schrödinger equation. However, for systems consisting of more than two interacting particles this is impossible analytically. It can only be achieved numerically and at exponentially increasing computational time costs with particle number.

A different type of solution to this problem is provided by Perturbation Theory. It splits the Hamiltonian describing the system into a solvable Hamiltonian which consists of a simplified version of the system whose determination is guaranteed by routinely used techniques in quantum mechanics and the rest of the Hamiltonian that makes solving the system a complicated problem, which is treated like a perturbation. The solution is then written as a power series in this perturbation. Every order in the perturbation is characterized by more and more complex terms which add to the previous solution. These terms are beautifully connected to physical processes that may take place in the system by the transparent formalism of Feynman diagrams.

The advantage of this method is that it consumes less computational time and can be applied to larger systems compared to exact methods. The perturbation expansion, even if limited to simple approximations still yields relevant results to scientific inquiries.

In the first chapter of this thesis, the basic principles of Many-body Perturbation Theory (MBPT) are explained. The second chapter shows how phenomena in the linear response theory of quantum systems can be understood also using MBPT. And finally, the third chapter presents examples of numerical calculations performed using algorithms based on MBPT methods and compares them with numerical calculations based on algorithms that solve the Schrödinger equation exactly.

1 Basics of Many-body Perturbation Theory

Introduction

In this section, the theoretical principles of Many-body Perturbation Theory applied to condensed matter physics are described. The first subsection contains the equilibrium Green's functions method for systems at zero temperature, whereas in the second subsection, the system still in equilibrium, is in contact with the environment at a finite temperature. Finally, in the last subsection, external fields and time-dependent perturbations are applied to the system, rendering necessary the use of nonequilibrium Green's functions.

1.1 Equilibrium Green's functions. Zero-temperature formalism

1.1.1 Fock space and field operators

In order to develop the tools to investigate many-particle phenomena, one needs to define a space of quantum states that consist of linear combinations of states with different number of particles, a collection of Hilbert spaces also known as Fock space.

Let $\{|\phi_{j,N}\rangle\}$ be a complete set of states in a N-particle Hilbert space. Then the Fock space is defined as the set of linear combinations of the form:[1]

$$|\psi\rangle = \alpha_0 |0\rangle + \sum_{N=1}^{\infty} \sum_{j=1}^{\infty} \alpha_j^N |\phi_{j,N}\rangle \quad (1.1)$$

An inner product can be defined as:

$$\langle\psi|\chi\rangle = \alpha_0^* \beta_0 + \sum_{N=1}^{\infty} \sum_{i,j=1}^{\infty} \alpha_j^{N*} \beta_i^N \langle\phi_{j,N}|\varphi_{i,N}\rangle \quad (1.2)$$

where:

$$|\chi\rangle = \beta_0 |0\rangle + \sum_{N=1}^{\infty} \sum_{j=1}^{\infty} \beta_j^N |\varphi_{j,N}\rangle \quad (1.3)$$

It follows from this definition that the inner product between states that contain different numbers of particles is zero. If the choice of basis in every Hilbert space is the N-particle ket vector in space-spin coordinates $\vec{x}_i = \{\vec{r}_i, \sigma_i\}$ then operators $\hat{\psi}^\dagger(\vec{x})$ that add particles at space-spin point \vec{x} and their adjoints which destroy particles, can be defined:

$$\hat{\psi}^\dagger(\vec{x}_1) \hat{\psi}^\dagger(\vec{x}_2) \dots \hat{\psi}^\dagger(\vec{x}_N) |0\rangle = |\vec{x}_1, \dots, \vec{x}_N\rangle \quad (1.4)$$

Throughout this thesis, systems to which the Fermi-Dirac statistics applies will be studied. Therefore:

$$|\dots \vec{x}_i, \dots, \vec{x}_j, \dots\rangle = -|\dots \vec{x}_j, \dots, \vec{x}_i, \dots\rangle \quad (1.5)$$

for any \vec{x}_i and \vec{x}_j .

In general, fermionic creation and annihilation field operators map wavefunctions from a n-particle Hilbert space to, respectively a n+1 and a n-1 particle Hilbert space:[1]

$$(\hat{\psi}^\dagger(\vec{x})\Psi_n)(\vec{x}_1, \dots, \vec{x}_{n+1}) \equiv \frac{(-1)^n}{\sqrt{n+1}} \sum_{j=1}^{n+1} (-1)^{j+1} \delta(\vec{x} - \vec{x}_j) \Psi_n(\vec{x}_1, \dots, \hat{x}_j, \dots, \vec{x}_{n+1}) \quad (1.6)$$

(\hat{x}_j denotes that this argument is missing)

$$(\hat{\psi}(\vec{x})\Psi_n)(\vec{x}_1, \dots, \vec{x}_{n-1}) \equiv \sqrt{n} \Psi_n(\vec{x}_1, \dots, \vec{x}_{n-1}, \vec{x}) \quad (1.7)$$

Fermionic field operators satisfy anticommutation relations:

$$\{\hat{\psi}^\dagger(\vec{x}), \hat{\psi}(\vec{x}')\} = \delta(\vec{x} - \vec{x}') \quad (1.8)$$

$$\{\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}')\} = 0 \quad (1.9)$$

$$\{\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{x}')\} = 0 \quad (1.10)$$

where anticommutation brackets are defined as:

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A} \quad (1.11)$$

The proof of these anticommutation relations is given in Appendix A.1.

Any one-body multiplicative or differential operator \hat{O} that is a sum of operators acting on each particle can be written in terms of field operators:

$$\hat{O} = \sum_i \hat{o}(\vec{x}_i) = \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{o}(\vec{x}) \hat{\psi}(\vec{x}) \quad (1.12)$$

Similarly, by deriving first the equality:

$$\hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) = \sum_{j \neq k}^n \delta(\vec{x} - \vec{x}_k) \delta(\vec{y} - \vec{x}_j) \quad (1.13)$$

the two-particle interaction can be rewritten:

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

For the derivation of the expressions of these operators in terms of field operators, see Appendix A.2. In conclusion, a general Hamiltonian of the form:

$$\hat{H}(t) = \sum_{i=1}^n \hat{h}(\vec{x}_i, t) + \frac{1}{2} \sum_{i \neq j}^n w(\vec{x}_i, \vec{x}_j) \quad (1.14)$$

can be re-expressed in terms of field operators as:

$$\hat{H}(t) = \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{h}(\vec{x}, t) \hat{\psi}(\vec{x}) + \frac{1}{2} \int d\vec{x} d\vec{y} w(\vec{x}, \vec{y}) \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \quad (1.15)$$

1.1.2 Three useful pictures from Quantum Mechanics

To analyze the time evolution of a quantum system, three descriptions within the quantum mechanics formalism proved useful in this study: the Schrödinger picture, the Interaction picture and the Heisenberg picture.

The Schrödinger picture

The usual framework of the Schrödinger equation corresponds to the Schrödinger picture where the state vectors depend on time and operators corresponding to observables do not.

$$i\hbar \partial_t |\Psi_S(t)\rangle = \hat{H} |\Psi_S(t)\rangle \quad (1.16)$$

Also because the focus of this subsection is equilibrium many-body theory, the Hamiltonian of the system is considered to be time-independent. The formal solution to this first-order differential equation is:

$$|\Psi_S(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar} |\Psi_S(t_0)\rangle \quad (1.17)$$

Therefore, the time evolution is generated by the Hamiltonian \hat{H}

The Interaction picture

The Interaction picture is half-way between the Schrödinger and the Heisenberg pictures. The key idea is to make the dichotomy $\hat{H} = \hat{H}_0 + \hat{V}$, where \hat{H}_0 represents the part of the Hamiltonian that results in a solvable problem, such as time-independent one-body operators, and \hat{V} represents the remaining part of the Hamiltonian, that makes solving the system a complicated problem. In the equilibrium case, \hat{V} is also time-independent. It can contain for example, two-body interaction operators.

Define:

$$|\Psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar} |\Psi_S(t)\rangle \quad (1.18)$$

which evolves as:

$$\begin{aligned} i\hbar\partial_t |\Psi_I(t)\rangle &= -\hat{H}_0 e^{i\hat{H}_0 t/\hbar} |\Psi_S(t)\rangle + e^{i\hat{H}_0 t/\hbar} (\hat{H}_0 + \hat{V}) |\Psi_S(t)\rangle \\ &= e^{i\hat{H}_0 t/\hbar} \hat{V} |\Psi_S(t)\rangle \\ &= e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0 t/\hbar} |\Psi_I(t)\rangle \end{aligned}$$

Therefore, in the Interaction picture, the following set of equations are valid:

$$i\hbar\partial_t |\Psi_I(t)\rangle = \hat{V}_I(t) |\Psi_I(t)\rangle \quad (1.19)$$

$$\hat{V}_I \equiv e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0 t/\hbar} \quad (1.20)$$

To keep the expectation values of operators picture-independent, one needs to define the operators in the Interaction picture in the following way:

$$\hat{O}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{O}_S e^{-i\hat{H}_0 t/\hbar} \quad (1.21)$$

Differentiating this definition with respect to time results in a useful equation of motion for the operators:

$$i\hbar\partial_t \hat{O}_I(t) = [\hat{O}_I(t), \hat{H}_0] \quad (1.22)$$

The time evolution operator in the Interaction picture

Define a unitary operator $\hat{U}(t, t_0)$ that makes the system evolve from time t_0 to time t :

$$|\Psi_I(t)\rangle = \hat{U}(t, t_0) |\Psi_I(t_0)\rangle \quad (1.23)$$

This operator has many interesting properties such as:[4]

$$\hat{U}(t, t) = 1 \quad (1.24)$$

$$\hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) = \hat{U}(t, t_0) \hat{U}^\dagger(t, t_0) = 1 \quad (1.25)$$

$$\hat{U}(t_1, t_2) \hat{U}(t_2, t_3) = \hat{U}(t_1, t_3) \quad (1.26)$$

$$\hat{U}(t_0, t) = \hat{U}^\dagger(t, t_0) \quad (1.27)$$

An integral equation for \hat{U} can be constructed which will be solved by iteration. From equations 1.19 and 1.23 it can be seen that \hat{U} satisfies a differential equation:

$$i\hbar\partial_t (\hat{U}(t, t_0) |\Psi_I(t_0)\rangle) = \hat{V}_I(t) \hat{U}(t, t_0) |\Psi_I(t_0)\rangle \quad (1.28)$$

Integrating this equation from t_0 to t yields:

$$\hat{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{V}_I(t') \hat{U}(t', t_0) \quad (1.29)$$

If \hat{U} were a function, this equation could be classified as a Volterra integral equation of the second kind:

$$\phi(x) = f(x) + \lambda \int_0^x K(x, u) \phi(u) du \quad (1.30)$$

and could be solved by means of the reciprocal kernel method[2]. Using the same algorithm as in [2], however always maintaining the proper ordering of the operators, yields a solution for \hat{U} of the following form:[3]

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \dots \int_{t_0}^t dt_n T[\hat{V}_I(t_1) \dots \hat{V}_I(t_n)] \quad (1.31)$$

(for details on the reciprocal kernel method and the detailed procedure for obtaining this solution, see Appendix A.3)

T stands for the time-ordered product of operators which orders the operators with the latest time to the left:[1]

$$T[\hat{A}_1(\bar{t}_1) \dots \hat{A}_n(\bar{t}_n)] = \sum_P (-1)^{F_P} \theta(\bar{t}_{P(1)}, \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)}, \bar{t}_{P(n)}) \\ \times \hat{A}_{P(1)}(\bar{t}_{P(1)}) \dots \hat{A}_{P(n)}(\bar{t}_{P(n)}) \quad (1.32)$$

where P runs over all permutations of the numbers $1 \dots n$ and F_P is the number of times a fermionic operator gets interchanged with another fermionic operator in the permutation P.

The Heisenberg picture

In the Heisenberg picture the state vectors do not depend on time, all the time dependence is in the operators. The state vector in the Heisenberg picture is defined as:

$$|\Psi_H(t)\rangle \equiv e^{i\hat{H}t/\hbar} |\Psi_S(t)\rangle \quad (1.33)$$

(\hat{H} here is time-independent because the equilibrium situation is in view)

From the definition it follows that:

$$i\hbar\partial_t |\Psi_H(t)\rangle = -e^{i\hat{H}t/\hbar} \hat{H} |\Psi_S(t)\rangle + e^{i\hat{H}t/\hbar} \hat{H} |\Psi_S(t)\rangle = 0 \quad (1.34)$$

This implies that $|\Psi_H(t)\rangle$ is time-independent.

To keep the expectation values of operators picture independent, a general operator in the Heisenberg picture needs to be defined in the following way:

$$\hat{O}_H \equiv e^{i\hat{H}t/\hbar} \hat{O}_S e^{-i\hat{H}t/\hbar} \quad (1.35)$$

Taking the time derivative of this definition yields:

$$i\hbar\partial_t \hat{O}_H(t) = [\hat{O}_H(t), \hat{H}] \quad (1.36)$$

All the three pictures coincide at $t=0$:

$$|\Psi_H\rangle = |\Psi_S(0)\rangle = |\Psi_I(0)\rangle \quad (1.37)$$

$$\hat{O}_S = \hat{O}_H(0) = \hat{O}_I(0) \quad (1.38)$$

In the Heisenberg picture, the state vectors satisfy the time-independent Schrödinger equation:

$$\hat{H} |\Psi_H\rangle = E |\Psi_H\rangle \quad (1.39)$$

and they represent the exact eigenstates of the system described by the full Hamiltonian \hat{H} . The fact that:

$$|\Psi_H\rangle = |\Psi_I(0)\rangle = \hat{U}(0, t_0) |\Psi_I(t_0)\rangle \quad (1.40)$$

helps construct these states from the interaction state vectors. The system described by \hat{H}_0 will be called noninteracting and its eigenstates are known.

Consider the time-dependent Hamiltonian:[4]

$$\hat{H}(t) = \hat{H}_0 + e^{-\epsilon|t|} \hat{V} \quad (1.41)$$

At very large times, both in the past and in the future, this Hamiltonian reduces to that of the noninteracting system (the system described by \hat{H}_0 , which is solvable) and at $t=0$, it becomes the full Hamiltonian \hat{H} that was used before in the definitions of the pictures and which describes the interacting system. If ϵ tends to zero at the end of the calculation, the perturbation is turned on and off infinitely slowly (adiabatically).

According to equation 1.40,

$$|\Psi_H\rangle = |\Psi_I(0)\rangle = \hat{U}_\epsilon(0, -\infty) |\phi_0\rangle \quad (1.42)$$

where ϕ_0 is a stationary eigenstate of the unperturbed Hamiltonian.

But one question remains: do meaningful results come out when the limit $\epsilon \rightarrow 0$ is taken? The answer to this question is provided by the Gell-Mann and Low theorem which prescribes the eigenstate that develops adiabatically from $|\phi_0\rangle$.

Theorem (Gell-Mann and Low). *If the following quantity exists to all orders in perturbation theory*

$$\lim_{\epsilon \rightarrow 0} \frac{\hat{U}_\epsilon(0, -\infty) |\phi_0\rangle}{\langle \phi_0 | \hat{U}_\epsilon(0, -\infty) |\phi_0\rangle} \equiv \frac{|\Psi_0\rangle}{\langle \phi_0 | \Psi_0\rangle} \quad (1.43)$$

then it is an eigenstate of \hat{H} :

$$\hat{H} \frac{|\Psi_0\rangle}{\langle \phi_0 | \Psi_0\rangle} = E \frac{|\Psi_0\rangle}{\langle \phi_0 | \Psi_0\rangle} \quad (1.44)$$

A simple proof[5] given by Luca Guido Molinary in his paper "Another proof of Gell-Mann and Low's theorem" is summarized in Appendix A.4.

Now one has all the necessary tools to introduce the concept of Green's functions and to proceed in the understanding of perturbation theory.

1.1.3 Green's functions. Diagrammatic analysis of perturbation theory

The definition of the single-particle Green's function is:[4]

$$iG_{\alpha\beta}(\vec{x}t, \vec{x}'t') = \frac{\langle \Psi_0 | T[\hat{\psi}_{H\alpha}(\vec{x}t) \hat{\psi}_{H\beta}^\dagger(\vec{x}'t')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (1.45)$$

where $|\Psi_0\rangle$ is the ground state of the interacting system, α, β are spin indices and $\vec{x}t$ represent the coordinates of a point in spacetime.

Why study such a quantity? Firstly, because the expectation value of any single-particle operator in the ground state of the system can be written in terms of the one-particle Green's function.

Proof. Let \hat{A} be the single-particle operator written in terms of field operators:

$$\hat{A} = \int d\vec{x} \sum_{\alpha\beta} \hat{\psi}_\beta^\dagger(\vec{x}) \hat{a}_{\beta\alpha}(\vec{x}) \hat{\psi}_\alpha(\vec{x}) \quad (1.46)$$

The ground state expectation value of \hat{A} is given by:

$$\langle \hat{A}_H(t) \rangle = \frac{\langle \Psi_0 | \hat{A}_H(t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (1.47)$$

$$= \sum_{\alpha\beta} \lim_{\vec{x}'t' \rightarrow \vec{x}t^+} \int d\vec{x} \frac{\langle \Psi_0 | \hat{\psi}_{H\beta}^\dagger(\vec{x}'t') \hat{a}_{\beta\alpha}(\vec{x}t) \hat{\psi}_{H\alpha}(\vec{x}t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (1.48)$$

$$= -i \int d\vec{x} \sum_{\alpha\beta} \lim_{\vec{x}'t' \rightarrow \vec{x}t^+} \hat{a}_{\beta\alpha}(\vec{x}) G_{\alpha\beta}(\vec{x}t, \vec{x}'t') \quad (1.49)$$

□

Secondly, the one-particle Green's function contains information on the ground-state energy of the system:[4]

$$E = \langle \hat{H} \rangle = -\frac{1}{2}i \int d\vec{x} \lim_{\vec{x}'t' \rightarrow \vec{x}t} \left(i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} \right) \sum_{\alpha\beta} G_{\alpha\beta}(\vec{x}t, \vec{x}'t') \quad (1.50)$$

Also there are many other interesting properties of the Green's function that make it worthwhile to calculate such as the fact that it can provide the excitation spectrum of the system (see Ref [1], subsection "Lehman representation").

Physically, the one-particle Green's function can be interpreted as the probability amplitude for the propagation of a particle or excitation between two spacetime points.[4]

Wick's theorem. Feynman diagrams

In order to determine the Green's function, it is necessary to write the Heisenberg field operators and the interacting ground state in its definition in terms of quantities easier to work with such as the ground state of the noninteracting system and operators in the interaction picture. It can be proven (see Appendix A.5) that:[4]

$$\begin{aligned} \frac{\langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} &= \frac{1}{\langle \phi_0 | \hat{U}_\epsilon(\infty, -\infty) | \phi_0 \rangle} \\ &\times \langle \phi_0 | \sum_{\nu=0}^{\infty} \left(-\frac{i}{\hbar} \right)^\nu \frac{1}{\nu!} \int_{-\infty}^{+\infty} dt_1 \dots \int_{-\infty}^{+\infty} dt_\nu e^{-\epsilon(|t_1| + \dots + |t_\nu|)} \\ &\times T[\hat{V}_I(t_1) \dots \hat{V}_I(t_\nu)] | \phi_0 \rangle \end{aligned} \quad (1.51)$$

Therefore, the Green's function can be written as:

$$\begin{aligned} iG_{\alpha\beta}(x, y) &= \sum_{\nu=0}^{\infty} \left(-\frac{i}{\hbar} \right)^\nu \frac{1}{\nu!} \int_{-\infty}^{+\infty} dt_1 \dots \int_{-\infty}^{+\infty} dt_\nu \\ &\times \frac{\langle \phi_0 | T[\hat{V}_I(t_1) \dots \hat{V}_I(t_\nu) \hat{\psi}_{I\alpha}(x) \hat{\psi}_{I\beta}^\dagger(y)] | \phi_0 \rangle}{\langle \phi_0 | \hat{U}_\epsilon(\infty, -\infty) | \phi_0 \rangle} \end{aligned} \quad (1.52)$$

(x, y are spacetime points)

The \hat{V}_I operators can also be written in terms of field operators in the interaction picture, therefore the problem of calculating the Green's function was reduced to that of evaluating expressions of the form: $\langle \phi_0 | T[\hat{\psi}_I^\dagger \dots \hat{\psi}_I] | \phi_0 \rangle$. The essential idea is to move all destruction operators to the right where they annihilate the noninteracting ground state.

In most systems of interest, $\hat{\psi}_I(x)$ can be uniquely separated into a destruction part $\hat{\psi}_I^{(+)}(x)$ that annihilates the noninteracting ground state and a creation part $\hat{\psi}_I^{(-)}(x)$, and similarly for $\hat{\psi}_I^\dagger(x)$:[3][4]

$$\hat{\psi}_I(x) = \hat{\psi}_I^{(+)}(x) + \hat{\psi}_I^{(-)}(x) \quad (1.53)$$

$$\hat{\psi}_I^{(+)}(x) | \phi_0 \rangle = 0 \quad (1.54)$$

$$\hat{\psi}_I^\dagger(x) = \hat{\psi}_I^{\dagger(+)}(x) + \hat{\psi}_I^{\dagger(-)}(x) \quad (1.55)$$

$$\hat{\psi}_I^{\dagger(-)}(x) | \phi_0 \rangle = 0 \quad (1.56)$$

The order of the field operators with all the destruction operators to the right and all the creation ones to the left is called normal order. The normal ordering symbol $N()$ places whatever operators it contains in normal order, also including a factor of (-1) for every interchange of fermionic operators. A normal ordered product of field operators is especially convenient because its expectation value in the unperturbed ground state $|\phi_0\rangle$ vanishes identically.

Thus the aim would be to reduce the T-product of field operators to a N-product. The quantity that remains after transforming a T-product of two operators into a normal ordering is called a contraction:

$$\overline{\hat{A}\hat{B}} \equiv T(\hat{A}\hat{B}) - N(\hat{A}\hat{B}) \quad (1.57)$$

For the case of two field operators, the only contractions that are non-zero are:

$$\langle \phi_0 | \overline{\hat{\psi}_I^{(+)}(x) \hat{\psi}_I^{\dagger(+)}(y)} | \phi_0 \rangle = \begin{cases} iG^0(x, y) & \text{if } t_x > t_y \\ 0 & \text{if } t_x < t_y \end{cases} \quad (1.58)$$

$$\langle \phi_0 | \overline{\hat{\psi}_I^{(-)}(x) \hat{\psi}_I^{\dagger(-)}(y)} | \phi_0 \rangle = \begin{cases} iG^0(x, y) & \text{if } t_y > t_x \\ 0 & \text{if } t_x > t_y \end{cases} \quad (1.59)$$

where $iG_{\alpha\beta}^0(x, y) = \langle \phi_0 | T[\hat{\psi}_{I\alpha}(x) \hat{\psi}_{I\beta}^{\dagger}(y)] | \phi_0 \rangle$ is a quantity which refers to the noninteracting system and is therefore calculable.

The generalization of what remains after the reduction of a T-product of arbitrary many fields to a normal ordering is known as Wick's theorem:

Theorem (Wick's theorem).

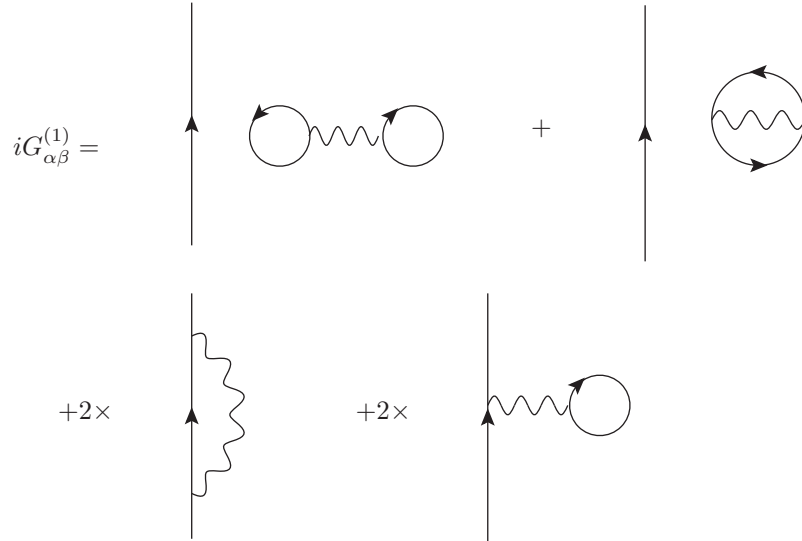
$$T[\hat{\psi}_I(x_1) \hat{\psi}_I^{\dagger}(x_2) \dots \hat{\psi}_I(x_n)] = N[\hat{\psi}_I(x_1) \hat{\psi}_I^{\dagger}(x_2) \dots \hat{\psi}_I(x_n) + \text{all possible contractions}] \quad (1.60)$$

For a proof using induction for Wick's theorem, see Appendix A.6. Wick's theorem makes possible the evaluation of the exact Green's function as an expansion involving only fully contracted field operators in the interaction picture. If G^0 is assigned a straight line with an arrow running from the second argument to the first, and the interaction potential a wavy line, the terms in the expansion, after applying Wick's theorem, can be represented graphically as Feynman diagrams.

For example, if one takes H_0 to describe a system of noninteracting particles and the perturbation adiabatically turned on to be the Coulomb interaction between particles:

$$\hat{V}_I(t) = \int d\vec{x}_1 \int d\vec{x}_2 V(\vec{x}_1, \vec{x}_2)_{\alpha\alpha'\beta\beta'} \delta(t_1 - t_2) \hat{\psi}_{I\alpha}^{\dagger}(x_1) \hat{\psi}_{I\beta}^{\dagger}(x_2) \hat{\psi}_{I\alpha'}(x_2) \hat{\psi}_{I\beta'}(x_1) \quad (1.61)$$

then, to first order in the interaction the numerator in the expression for the Green's function (equation 1.52) can be written as a sum of Feynman diagrams in the following way:



It can be proven (see proof in Appendix A.7) that the disconnected diagrams (the ones containing separated pieces) factor out from the numerator of equation 1.52 and exactly cancel the denominator, leaving the following expression for G:

$$iG_{\alpha\beta}(x, y) = \sum_{\nu=0}^{\infty} \left(-\frac{i}{\hbar}\right)^{\nu} \frac{1}{\nu!} \int_{-\infty}^{+\infty} dt_1 \dots \int_{-\infty}^{+\infty} dt_{\nu} \times \langle \phi_0 | T[\hat{V}_I(t_1) \dots \hat{V}_I(t_{\nu}) \hat{\psi}_{I\alpha}(x) \hat{\psi}_{I\beta}^{\dagger}(y)] | \phi_0 \rangle_{\text{connected}} \quad (1.62)$$

In conclusion, for this case, the Feynman rules that enable one to write the n^{th} order contribution to the single particle Green's function can be enumerated:[4]

1. Draw all topologically distinct connected diagrams with n interaction lines and $2n+1$ directed particle Green's functions lines.
2. Label each vertex with a four-dimensional spacetime point x_i
3. Assign to each wavy line an interaction:

$$U(x, y)_{\lambda\lambda'\mu\mu'} = V(\vec{x}, \vec{y})_{\lambda\lambda'\mu\mu'} \delta(t_x - t_y) \quad (1.63)$$

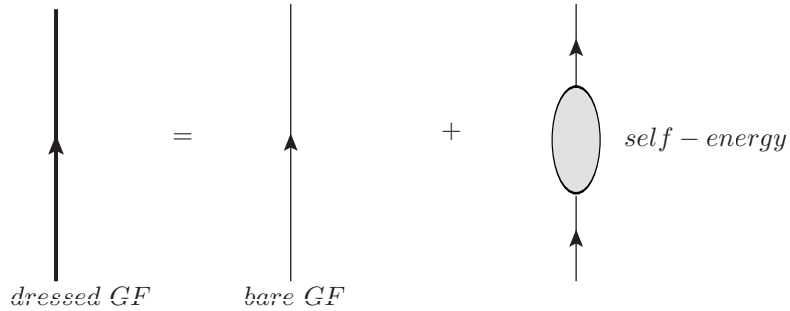
4. Assign to each solid line a Green's function $G_{\alpha\beta}^0(x, y)$.
5. Integrate all internal variables over space and time.
6. There is a spin-matrix product along each continuous fermion line, including the potential at each vertex.
7. Affix a sign factor $(-1)^F$ to each term, where F is the number of closed fermion loops in the diagram and a factor $(\frac{i}{\hbar})^n$ to each n^{th} order term.

Dyson's equation

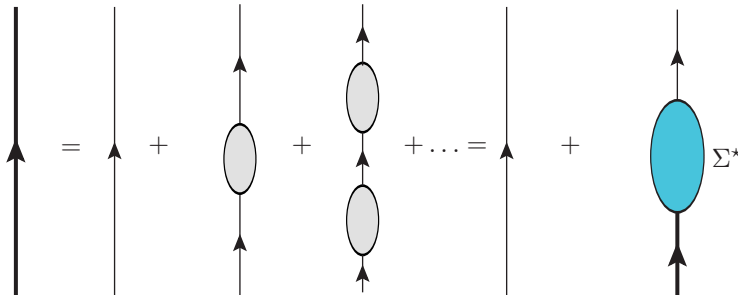
In practise however, the bare Green's functions G^0 are never used to expand the diagrams in. Instead, self consistent equations involving the dressed Green's functions are used. This has the advantage of dealing with physical, renormalized Green's functions and also a smaller number of diagrams is needed. An example of such an equation is Dyson's equation which is the subject of this subsection.

The conclusion of the previous subsection was that the exact Green's function consists of the unperturbed Green's function plus all connected diagrams with a free Green's function at each end.

Define a self-energy insertion as any part of a diagram that is connected to the rest of the diagram by two particle lines:



Also define a proper self-energy insertion as a self-energy insertion that cannot be separated into two pieces by cutting a single particle line. The proper self energy Σ^* is the sum of all proper self-energy insertions.



In terms of these newly defined quantities, an integral equation for the exact Green's function can be written:

$$G_{\alpha\beta}(x, y) = G_{\alpha\beta}^0(x, y) + \int dx_1 \int dx_1' G_{\alpha\lambda}^0(x, x_1) \Sigma^*(x_1, x_1')_{\lambda\mu} G_{\mu\beta}(x_1', y) \quad (1.64)$$

This is called Dyson's equation and it can be solved iteratively. The power of this equation lies in the fact that any approximation for Σ^* generates an infinite-order approximate series for the Green's function, thus making possible the summation of an infinite class of perturbation terms.

1.2 Equilibrium finite temperature formalism

So far, the system which was intended to be studied using perturbation theory was considered isolated. In reality, however, a system is always coupled to an environment with which it exchanges energy and mass until a state of equilibrium is reached. In this part, the Green's functions formalism is upgraded so that it enables the calculation of expectation values of observables concerning a system in thermodynamical equilibrium with an external reservoir with respect to both particle and energy exchange.

1.2.1 Prelude in statistical physics

Consider first a case in classical mechanics, a macroscopic system containing a large number of particles and assume that it is closed, i.e. it does not interact with other systems. A part of the system which is very small compared to the whole system, but still macroscopic, is called a subsystem. It is not closed, it interacts in complex ways with the other parts of the system, rendering the usual calculation methods of mechanics inapplicable. The methods of statistical physics will be used instead.

An observation which this new approach is based on is that after a sufficiently long time, the subsystem will have been many times in every possible state.[6] Let Δt be the part of the total time T during which the subsystem was in a given volume of phase space $\Delta p \Delta q$. Then, the quantity:

$$w = \lim_{T \rightarrow \infty} \frac{\Delta t}{T} \quad (1.65)$$

represents the probability that if the subsystem is observed at an arbitrary instant in time, it will be found in the given volume of phase space $\Delta p \Delta q$. This probability can be written as:

$$dw = \rho(p_1 \dots p_s, q_1 \dots q_s) dp dq \quad (1.66)$$

where ρ is a function of the coordinates and momenta corresponding to the s degrees of freedom of the system. This function is called the probability density or the statistical distribution function and its determination is the fundamental problem of statistical physics. If this problem is solved, it becomes possible to calculate the probabilities to obtain the values upon measurement of any physical quantity related to the subsystem, $f(p, q)$, by multiplying each of its possible values by the probability density and integrating over all states:

$$\bar{f} = \int f(p, q) \rho(p, q) dp dq \quad (1.67)$$

The averaging with respect to the distribution function (statistical averaging) is equivalent to a time averaging as can be seen from equation 1.65

Now going back to quantum mechanics, the situation is similar to that of the macroscopic body in the sense that many-body quantum systems have an extremely high density of levels in the energy eigenvalue spectrum. As it is impossible in classical mechanics to take into account the initial conditions for every particle in a body, it is impossible to find a wavefunction to describe a complex interacting many-particle quantum system.

Extrapolating equation 1.67 yields for the expectation value of a quantum mechanical operator acting on a quantum system in equilibrium with its environment:

$$\langle \hat{A} \rangle = \sum_n p_n \langle n | \hat{A} | n \rangle \quad (1.68)$$

where $|n\rangle$ are the eigenstates obtained by solving the system when all interactions with the surrounding environment of the system are not taken into account and p_n is the probability of finding the interacting system in the state $|n\rangle$ at a given time.

Birkhoff's ergodic theorem shows that the probabilities p_n can be understood in a different way in which the time averaging is equivalent to an ensemble averaging. Instead of investigating the state of the system at many various times and taking the average, one can prepare a large number of identical systems which have reached equilibrium and at a given instant of time t_0 , one counts M_n of the M systems to be in the state n . Then p_n is given by:

$$p_n = \frac{M_n}{M} \quad (1.69)$$

In conclusion, a grand canonical ensemble is an imaginary collection of model systems put together to mirror the calculated probability distribution of a given system (the amount of members of the ensemble which are in the microscopic state i is proportional to the probability over time of finding the real-world system in that microscopic state i).

If $|\Psi_k\rangle$ is a complete orthonormal set of states in the system Hilbert space, then:

$$\langle \hat{A} \rangle = \sum_n p_n \langle n | \hat{A} | n \rangle \quad (1.70)$$

$$= \sum_{n,k} p_n \langle n | \hat{A} | \Psi_k \rangle \langle \Psi_k | n \rangle \quad (1.71)$$

$$= \sum_n p_n \langle \Psi_k | n \rangle \langle n | \hat{A} | \Psi_k \rangle \quad (1.72)$$

$$= \sum_k \langle \Psi_k | \hat{\rho} \hat{A} | \Psi_k \rangle \quad (1.73)$$

$$= Tr\{\hat{\rho} \hat{A}\} \quad (1.74)$$

where the density operator $\hat{\rho}$ was defined as:

$$\hat{\rho} = \sum_n p_n |n\rangle \langle n| \quad (1.75)$$

and the trace $Tr\{\hat{A}\}$ of an operator is defined as:

$$Tr\{\hat{A}\} = \sum_k \langle \Psi_k | \hat{A} | \Psi_k \rangle \quad (1.76)$$

The next step is to determine the density matrix operator $\hat{\rho}$ for equilibrium systems. This derivation follows the derivation given in reference [7].

Assuming that the total hypersystem made out of the M identical systems has total energy E and fixed particle number N , then:

$$E = \sum_n M_n E_n \quad (1.77)$$

$$N = \sum_n M_n N_n \quad (1.78)$$

The degeneracy of the energy level E , denoted by Ω can be calculated to be:

$$\Omega = \frac{M!}{M_1! \dots M_n!} \quad (1.79)$$

further yielding:

$$\ln \Omega = \ln M! - \sum_n \ln M_n! \quad (1.80)$$

$$= M \ln M - M - \sum_n (M_n \ln M_n - M_n) \quad (1.81)$$

$$= -M \sum_n p_n \ln p_n \quad (1.82)$$

$$= MS \quad (1.83)$$

where the quantity $S = -\sum_n p_n \ln p_n$ will be called the entropy.

The most probable configuration of the ensemble is the one which maximizes the degeneracy of the level E and therefore, the entropy. The constraints are:

$$\sum_n p_n = 1 \quad (1.84)$$

$$E_S = \frac{E}{M} = \frac{\sum_n M_n E_n}{M} = \sum_n p_n E_n \quad (1.85)$$

$$N_S = \frac{N}{M} = \frac{\sum_n M_n N_n}{M} = \sum_n p_n N_n \quad (1.86)$$

where E_S and N_S are the expectation values of the energy and number of particles of each system in the ensemble.

The Lagrange multipliers method can be applied:

$$\begin{aligned} \Lambda(p_n, \alpha, \beta, \gamma) = & - \sum_n p_n \ln p_n - \alpha \left(\sum_n p_n N_n - N_S \right) \\ & - \beta \left(\sum_n p_n E_n - E_S \right) - \gamma \left(\sum_n p_n - 1 \right) \end{aligned}$$

$d\Lambda = 0$ implies $\frac{d\Lambda}{dp_n} = 0$ which gives:

$$-(\ln p_n + 1) - \alpha N_n - \beta E_n - \gamma = 0 \quad (1.87)$$

$$\ln p_n = -1 - \alpha N_n - \beta E_n - \gamma \quad (1.88)$$

$$p_n = e^{-(\gamma+1)} \cdot e^{-\alpha N_n - \beta E_n} \quad (1.89)$$

Replacing equation 1.89 in equation 1.84 yields:

$$\frac{1}{e^{\gamma+1}} \sum_n e^{-\alpha N_n - \beta E_n} = 1 \quad (1.90)$$

Denote:

$$\sum_n e^{-\alpha N_n - \beta E_n} = Z \quad (1.91)$$

which means:

$$e^{-(\gamma+1)} = \frac{1}{Z} \quad (1.92)$$

and

$$p_n = \frac{1}{Z} e^{-\alpha N_n - \beta E_n} \quad (1.93)$$

Rewriting the entropy:

$$\begin{aligned} S = - \sum_n p_n \ln p_n &= \sum_n p_n (1 + \alpha N_n + \beta E_n + \gamma) \\ &= \sum_n p_n + \alpha \sum_n p_n N_n + \beta \sum_n p_n E_n + \gamma \sum_n p_n \\ &= 1 + \alpha N_S + \beta E_S + \gamma \end{aligned}$$

Using equation 1.92 in the form $1 + \gamma = \ln Z$ yields for the entropy:

$$S = \alpha N_S + \beta E_S + \ln Z \quad (1.94)$$

Taking the partial derivatives with respect to E_S and N_S of the entropy:

$$\frac{\partial S}{\partial E_S} = \beta + E_S \frac{\partial \beta}{\partial E_S} + N_S \frac{\partial \alpha}{\partial E_S} + \frac{\partial(\ln Z)}{\partial E_S} \quad (1.95)$$

$$\frac{\partial S}{\partial N_S} = \frac{\partial \beta}{\partial N_S} E_S + \alpha + \frac{\partial \alpha}{\partial N_S} N_S + \frac{\partial(\ln Z)}{\partial N_S} \quad (1.96)$$

Now,

$$\frac{\partial(\ln Z)}{\partial E_S} = \frac{\partial(\ln Z)}{\partial \beta} \frac{\partial \beta}{\partial E_S} + \frac{\partial(\ln Z)}{\partial \alpha} \frac{\partial \alpha}{\partial E_S} \quad (1.97)$$

It is straightforward to obtain:

$$\frac{\partial(\ln Z)}{\partial\beta} = -E_S \quad (1.98)$$

$$\frac{\partial(\ln Z)}{\partial\alpha} = -N_S \quad (1.99)$$

which, when replaced in equation 1.97 and then in 1.96 will give the simple result:

$$\frac{\partial S}{\partial E_S} = \beta \quad (1.100)$$

Analogously,

$$\frac{\partial S}{\partial N_S} = \alpha \quad (1.101)$$

Defining the temperature T and the chemical potential μ of the system with the relations:

$$\frac{1}{T} = \frac{\partial S}{\partial E_S} \quad (1.102)$$

$$-\frac{\mu}{T} = \frac{\partial S}{\partial N_S} \quad (1.103)$$

yields:

$$\beta = \frac{1}{T} \quad (1.104)$$

$$\alpha = -\beta\mu \quad (1.105)$$

and

$$p_n = \frac{1}{Z} e^{-\beta(E_n - \mu N_n)} \quad (1.106)$$

Then

$$\hat{\rho} = \sum_n p_n |n\rangle\langle n| = \frac{1}{Z} e^{-\beta(E_n - \mu N_n)} |n\rangle\langle n| \quad (1.107)$$

The action of $\hat{\rho}$ on a state $|n\rangle$ is:

$$\hat{\rho}|n\rangle = \frac{1}{Z} e^{-\beta(E_n - \mu N_n)} |n\rangle \quad (1.108)$$

which motivates writing $\hat{\rho}$ as:

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu\hat{N})} \quad (1.109)$$

And Z can be written also in terms of operators as:

$$\begin{aligned} Z &= \sum_n e^{-\beta(E_n - \mu N_n)} = \langle n| \sum_n e^{-\beta(\hat{H} - \mu\hat{N})} |n\rangle \\ &= Tr \left\{ e^{-\beta(\hat{H} - \mu\hat{N})} \right\} \end{aligned}$$

Z is called the grand partition function. In terms of this expression for Z , the density operator is:

$$\hat{\rho} = \frac{e^{-\beta(\hat{H} - \mu\hat{N})}}{Tr \left\{ e^{-\beta(\hat{H} - \mu\hat{N})} \right\}} \quad (1.110)$$

1.2.2 Temperature Green's functions

In this paragraph, the considerations derived from studying a system in equilibrium with the environment will be applied to deduce how perturbation theory methods for the ground state formalism should be extended to the finite temperature case.

Defining the grand canonical Hamiltonian as:

$$\hat{K} = \hat{H} - \mu\hat{N} \quad (1.111)$$

with the same dichotomy as previously:

$$\hat{K} = \hat{K}_0 + \hat{K}' \quad (1.112)$$

where \hat{K}_0 represents the solvable part, a modified Heisenberg picture can be introduced:

$$\hat{O}_K(\vec{x}\tau) \equiv e^{i\hat{K}\tau/\hbar} \hat{O}_S(\vec{x}) e^{-i\hat{K}\tau/\hbar} \quad (1.113)$$

Field operators can be constructed for this picture:

$$\hat{\psi}_{K\alpha}(\vec{x}\tau) = e^{i\hat{K}\tau/\hbar} \hat{\psi}_\alpha(\vec{x}) e^{-i\hat{K}\tau/\hbar} \quad (1.114)$$

$$\hat{\psi}_{K\alpha}^\dagger(\vec{x}\tau) = e^{i\hat{K}\tau/\hbar} \hat{\psi}_\alpha^\dagger(\vec{x}) e^{-i\hat{K}\tau/\hbar} \quad (1.115)$$

The single particle temperature Green's function is defined as:[4]

$$\mathcal{G}_{\alpha\beta}(\vec{x}\tau, \vec{x}'\tau') = -Tr \left\{ \hat{\rho} T_\tau [\hat{\psi}_{K\alpha}(\vec{x}\tau) \hat{\psi}_{K\beta}^\dagger(\vec{x}'\tau')] \right\} \quad (1.116)$$

The same relations to observables apply as in the case of zero-temperature formalism.

Perturbation theory and Wick's theorem for finite temperatures

For any operator \hat{O}_S in the Schrödinger picture, an operator in the interaction picture can formally be defined as:[4]

$$\hat{O}_I(\tau) \equiv e^{i\hat{K}_0\tau/\hbar} \hat{O}_S(\vec{x}) e^{-i\hat{K}_0\tau/\hbar} \quad (1.117)$$

The Heisenberg operators and the interaction picture operators are related by the equation:

$$\hat{O}_K(\tau) = e^{i\hat{K}\tau/\hbar} e^{-i\hat{K}_0\tau/\hbar} \hat{O}_I(\tau) e^{i\hat{K}_0\tau/\hbar} e^{-i\hat{K}\tau/\hbar} \quad (1.118)$$

$$= \hat{U}(0, \tau) \hat{O}_I(\tau) \hat{U}(\tau, 0) \quad (1.119)$$

where the operator \hat{U} is defined by:

$$\hat{U}(\tau_1, \tau_2) \equiv e^{i\hat{K}_0\tau_1/\hbar} e^{-i\hat{K}(\tau_1-\tau_2)/\hbar} e^{-i\hat{K}_0\tau_2/\hbar} \quad (1.120)$$

A differential equation for \hat{U} can be obtained:

$$-i \frac{\partial}{\partial \tau} \hat{U}(\tau, \tau') = \frac{\partial}{\partial \tau} \left(e^{i\hat{K}_0\tau/\hbar} e^{-i\hat{K}(\tau-\tau')/\hbar} e^{-i\hat{K}_0\tau'/\hbar} \right) \quad (1.121)$$

$$= e^{i\hat{K}_0\tau/\hbar} (\hat{K}_0 - \hat{K}) e^{-i\hat{K}(\tau-\tau')/\hbar} e^{-i\hat{K}_0\tau'/\hbar} \quad (1.122)$$

$$= e^{i\hat{K}_0\tau/\hbar} (\hat{K}_0 - \hat{K}) e^{-i\hat{K}_0\tau/\hbar} \hat{U}(\tau, \tau') \quad (1.123)$$

$$= -\hat{K}'_I \hat{U}(\tau, \tau') \quad (1.124)$$

The equation

$$\frac{\partial}{\partial \tau} \hat{U}(\tau, \tau') = \left(-\frac{i}{\hbar} \right) \hat{K}'_I \hat{U}(\tau, \tau') \quad (1.125)$$

is of the same kind as the one that was solved for the time evolution operator in the ground state formalism, therefore using the same algorithm described in Appendix A.3 yields the solution:

$$\hat{U}(\tau, \tau') = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \dots \int_{\tau'}^{\tau} d\tau_n \times T_\tau \left[\hat{K}'_I(\tau_1) \dots \hat{K}'_I(\tau_n) \right] \quad (1.126)$$

From equation 1.120, if $\tau_2 = 0, \tau_1 = \tau$ then

$$e^{-i\hat{K}\tau/\hbar} = e^{-i\hat{K}_0\tau/\hbar}\hat{\mathcal{U}}(\tau, 0) \quad (1.127)$$

If $\tau = -i\beta\hbar$, a perturbation expansion for ρ can also be obtained.

$$\hat{\rho} = \frac{e^{-\beta\hat{K}}}{Tr\{e^{-\beta\hat{K}}\}} \quad (1.128)$$

and

$$\hat{\rho}_0 = \frac{e^{-\beta\hat{K}_0}}{Tr\{e^{-\beta\hat{K}_0}\}} \quad (1.129)$$

Therefore, τ will be considered a time variable running on the imaginary axis.

The exact temperature Green's function can be rewritten as:

$$\mathcal{G}_{\alpha\beta}(\vec{x}\tau, \vec{x}'\tau') = -\frac{Tr\{e^{-\beta\hat{K}_0}\hat{\mathcal{U}}(-i\beta\hbar, 0)\hat{\mathcal{U}}(0, \tau)\hat{\psi}_{I\alpha}(\vec{x}\tau)\hat{\mathcal{U}}(\tau, \tau')\hat{\psi}_{I\beta}^\dagger(\vec{x}'\tau')\hat{\mathcal{U}}(\tau', 0)\}}{Tr\{e^{-\beta\hat{K}_0}\hat{\mathcal{U}}(-i\beta\hbar, 0)\}} \quad (1.130)$$

for $|\tau| > |\tau'|$.

Using equation 1.126 for the time-evolution operators yields:

$$\begin{aligned} \mathcal{G}_{\alpha\beta}(\vec{x}\tau, \vec{x}'\tau') &= -Tr\{e^{-\beta\hat{K}_0} \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{-i\beta\hbar}^0 d\tau_1 \dots \int_{-i\beta\hbar}^0 d\tau_n \\ &\times Tr\left[\hat{K}'_I(\tau_1) \dots \hat{K}'_I(\tau_n)\hat{\psi}_{I\alpha}(\vec{x}\tau)\hat{\psi}_{I\beta}^\dagger(\vec{x}'\tau')\right]\} \\ &\times \frac{1}{Tr\{e^{-\beta\hat{K}_0} \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{-i\beta\hbar}^0 d\tau_1 \dots \int_{-i\beta\hbar}^0 d\tau_n Tr\left[\hat{K}'_I(\tau_1) \dots \hat{K}'_I(\tau_n)\right]\}} \end{aligned} \quad (1.131)$$

The denominator serves to eliminate all disconnected diagrams as in the zero-temperature formalism.

The next step in the zero-temperature case was to turn the time ordered products into normal ordered ones because their ground state expectation value vanished. However, the ensemble average of the normal product is not zero. Nevertheless, as first proved by T. Matsubara, there exists a generalized Wick's theorem that allows a diagrammatic expansion of the temperature Green's function[4]. Firstly, the noninteracting temperature Green's function is:

$$\mathcal{G}_{\alpha\beta}^0(\vec{x}\tau, \vec{x}'\tau') = -Tr\left\{\hat{\rho}_0 Tr_\tau[\hat{\psi}_{I\alpha}(\vec{x}\tau)\hat{\psi}_{I\beta}^\dagger(\vec{x}'\tau')]\right\} \quad (1.132)$$

where

$$\hat{\rho} = \frac{e^{-\beta\hat{K}_0}}{Tr\{e^{-\beta\hat{K}_0}\}} \quad (1.133)$$

Define a contraction as:

$$\overline{\hat{A}\hat{B}} = Tr\{\hat{\rho}_0 Tr_\tau[\hat{A}\hat{B}]\} \quad (1.134)$$

For example,

$$\overline{\hat{\psi}_{I\alpha}(\vec{x}\tau)\hat{\psi}_{I\beta}^\dagger(\vec{x}'\tau')} = -\mathcal{G}_{\alpha\beta}^0(\vec{x}\tau, \vec{x}'\tau') \quad (1.135)$$

Theorem (The generalized Wick's theorem).

$$Tr\{\hat{\rho}_0 Tr_\tau[\hat{A}\hat{B}\hat{C} \dots \hat{Z}]\} = \text{the sum over all possible fully contracted terms}$$

where $\hat{A}, \hat{B}, \dots, \hat{Z}$ are field operators in the interaction picture.

The proof of the generalized Wick theorem can be found in Appendix A.8.

Since the algebraic structure of the finite temperature Wick's theorem is identical to that of the fully contracted terms in the zero-temperature form, the Green's function \mathcal{G} has the same set of Feynman diagrams that G had at zero temperature.

Feynman rules

If \hat{H}' is taken to be the two particle interaction:

$$\hat{K}' = \hat{H}' = \frac{1}{2} \int d\vec{x}_1 d\vec{x}_2 V(\vec{x}_1, \vec{x}_2) \hat{\psi}_\alpha^\dagger(\vec{x}_1) \hat{\psi}_\beta^\dagger(\vec{x}_2) \hat{\psi}_\beta(\vec{x}_2) \hat{\psi}_\alpha(\vec{x}_1) \quad (1.136)$$

the corresponding interaction-picture operator being:

$$\hat{K}_I(\tau_1) = \frac{1}{2} \int d\vec{x}_1 d\vec{x}_2 \int_{-i\beta\hbar}^0 \hat{\psi}_{I\alpha}^\dagger(\vec{x}_1\tau_1) \hat{\psi}_{I\beta}^\dagger(\vec{x}_2\tau_2) \mathcal{V}_0(\vec{x}_1\tau_1, \vec{x}_2\tau_2) \hat{\psi}_{I\beta}(\vec{x}_2\tau_2) \hat{\psi}_{I\alpha}(\vec{x}_1\tau_1) \quad (1.137)$$

where:

$$\mathcal{V}_0(\vec{x}_1\tau_1, \vec{x}_2\tau_2) = V(\vec{x}_1 - \vec{x}_2) \delta(\tau_1 - \tau_2) \quad (1.138)$$

the following Feynman rules can be written down:

1. Draw all topologically distinct connected diagrams with n interaction lines and $2n+1$ directed particle Green's functions lines.
2. Assign to each wavy line an interaction: $\mathcal{V}_0(1, 2)$
3. Associate a factor $\mathcal{G}_{\alpha\beta}^0(1, 2)$ with each directed particle line running from spacetime point 2 to spacetime point 1.
4. Integrate all internal variables: $\int d\vec{x}_i \int_{-i\beta\hbar}^0 d\tau_i$.
5. There is a spin-matrix product along each continuous fermion line, including the potential at each vertex.
6. Affix a sign factor $(-1)^F$ to each term, where F is the number of closed fermion loops in the diagram and a factor $\left(\frac{-i}{\hbar}\right)^n$ to each n^{th} order term.
7. Interpret any temperature Green's function at equal values of τ as:
 $\mathcal{G}^0(\vec{x}\tau, \vec{x}'\tau) = \lim_{\tau' \rightarrow \tau^+} \mathcal{G}^0(\vec{x}\tau, \vec{x}'\tau')$

Also, the temperature Green's function obeys Dyson's equation:

$$\mathcal{G}(1, 2) = \mathcal{G}^0(1, 2) + \int d3d4 \mathcal{G}(1, 3) \Sigma^*(3, 4) \mathcal{G}(4, 2) \quad (1.139)$$

This concludes the discussion about equilibrium Green's functions where the Hamiltonian of the system was time independent. A new challenge awaits, that of subjecting the system to a time-independent perturbation such as an external field or a laser pulse and investigating it using many-body perturbation theory. This will be the subject of the remaining part of this thesis.

1.3 Non-equilibrium finite temperature formalism

In this section, the goal of study is extended to describing many-electron systems that are initially in thermal equilibrium and are afterwards subjected to time-dependent external fields.

The Hamiltonian has now a more general, time-dependent expression:

$$\hat{H}(t) = \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{h}(\vec{x}, t) \hat{\psi}(\vec{x}) + \frac{1}{2} \int d\vec{x} d\vec{y} w(\vec{x}, \vec{y}) \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \quad (1.140)$$

with:

$$\hat{h}(\vec{x}, t) = \frac{1}{2} \left(-i\nabla + \vec{A}(\vec{x}, t) \right)^2 + v(\vec{x}, t) - \mu \quad (1.141)$$

The external potential $v(\vec{x}, t)$ and the vector potential $\vec{A}(\vec{x}, t)$ are switched on at $t = t_0$. For $t < t_0$ the Hamiltonian is time-independent as was the case in the previous subsection.

The time evolution operator $\hat{U}(t, t')$ is defined by:

$$|\Psi(t)\rangle = \hat{U}(t, t') |\Psi(t')\rangle \quad (1.142)$$

where $|\Psi(t)\rangle$ is a solution of the time-dependent Schrödinger equation:

$$(i\partial_t - \hat{H}(t))\Psi(\vec{x}_1, \dots, \vec{x}_n, t) = 0 \quad (1.143)$$

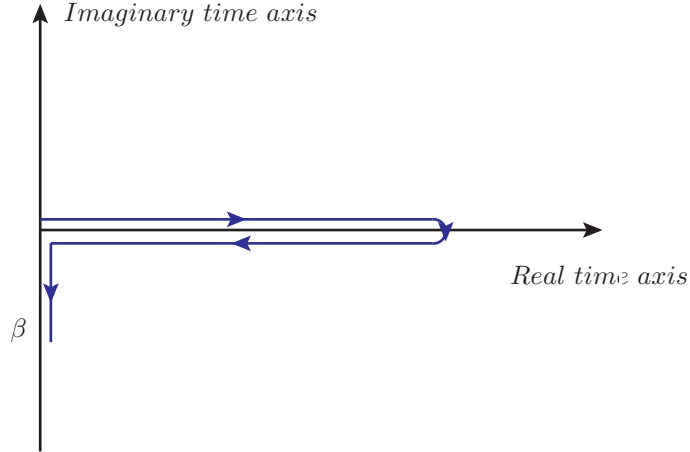
(in this part, atomic units will be used) The expectation value of an operator \hat{O} at time t will have a similar expression as in the finite temperature case:

$$\langle \hat{O}_H(t) \rangle = Tr\{\hat{\rho}\hat{O}_H(t)\} \quad (1.144)$$

The difference resides in the fact that $\hat{\rho}$ and the time evolution operator \hat{U} in the expression of $\hat{O}_H(t) = \hat{U}(t_0, t)\hat{O}\hat{U}(t, t_0)$ are built out of different Hamiltonians, therefore requiring two different perturbation expansions. In order to avoid this, an alternative mathematical approach can be adopted. ([1][8]) If $\hat{H}(t)$ is defined to be equal to \hat{H}_0 (the time-independent part of the Hamiltonian) on the contour running straight from t_0 to $t_0 - i\beta$ in the complex time plane, then:

$$\langle \hat{O}(t) \rangle = \frac{Tr\left\{\hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t)\hat{O}\hat{U}(t, t_0)\right\}}{Tr\left\{\hat{U}(t_0 - i\beta, t_0)\right\}} \quad (1.145)$$

Reading the time arguments of the evolution operators in order, suggests that the system formally evolves along the real time axis from t_0 to t after which the operator \hat{O} acts. Then it evolves back along the real time axis to t_0 and, in the end, along the imaginary time axis to $t_0 - i\beta$. This path is called the Keldysh contour:



Turning the usual time integrals in the expression for the time evolution operator:

$$\hat{U}(t, t') = T[\exp(-i \int_{t'}^t d\tau, \hat{H}(\tau))] \quad (1.146)$$

into contour integrals, both the actions of $\hat{\rho}$ and \hat{H} can be included in the expansion of \hat{U} , yielding in a similar fashion as in the equilibrium formalism:

$$\langle \hat{O}_H(t) \rangle = \frac{Tr\left\{T_c[\exp(-i \int_c d\bar{t}, \hat{H}(\bar{t}))\hat{O}(t)]\right\}}{Tr\left\{T_c[\exp(-i \int_c d\bar{t}, \hat{H}(\bar{t}))]\right\}} \quad (1.147)$$

where the contour ordered product of operators is defined as:

$$T_c[\hat{A}_1(\bar{t}_1) \dots \hat{A}_n(\bar{t}_n)] = \sum_P (-1)^{F_P} \theta(\bar{t}_{P(1)}, \bar{t}_{P(2)}) \dots \theta(\bar{t}_{P(n-1)}, \bar{t}_{P(n)}) \\ \times \hat{A}_{P(1)}(\bar{t}_{P(1)}) \dots \hat{A}_{P(n)}(\bar{t}_{P(n)}) \quad (1.148)$$

$\theta(t_1, t_2)$ is generalized for arguments on the contour:

$$\theta(t_1, t_2) = \begin{cases} 1 & \text{if } t_1 \text{ is later on the contour than } t_2, \\ 0 & \text{otherwise.} \end{cases}$$

This expression can also be used to generate a diagrammatic analysis of the Green's function after applying a generalized Wick's theorem (see reference [9]). Here, for completeness, a functional derivatives approach will be described which although formally slightly different, reaches the same equations of motion for the Green's function as the previous method adjusted for the non-equilibrium case would, namely, the Kadanoff-Baym equations. The presentation of this approach follows reference [1] Define now, the one-particle non-equilibrium Green's function as:

$$G(1, 2) = -i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) T_c [\hat{\psi}_H(1) \hat{\psi}_H^\dagger(2)] \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \quad (1.149)$$

$$= -i \langle T_c [\hat{\psi}_H(1) \hat{\psi}_H^\dagger(2)] \rangle \quad (1.150)$$

Also:

$$G(1, 2) = \theta(t_1, t_2) G^>(1, 2) + \theta(t_2, t_1) G^<(1, 2) \quad (1.151)$$

with:

$$G^>(1, 2) = -i \langle \hat{\psi}_H(1) \hat{\psi}_H^\dagger(2) \rangle \quad (1.152)$$

$$G^<(1, 2) = i \langle \hat{\psi}_H^\dagger(2) \hat{\psi}_H(1) \rangle \quad (1.153)$$

($i=(\vec{x}_i t_i)$)

The starting point in obtaining an equation of motion for the Green's function is the equations of motion for the field operators:

$$i\partial_{t_1} \hat{\psi}_H(\vec{x}_1 t_1) = \left[\hat{\psi}(\vec{x}_1), \hat{H}(t_1) \right]_H \quad (1.154)$$

$$\begin{aligned} &= \left[\hat{\psi}(\vec{x}_1), \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{h}(\vec{x}, t_1) \hat{\psi}(\vec{x}) \right]_H \\ &+ \frac{1}{2} \left[\hat{\psi}(\vec{x}_1), \int d\vec{x} d\vec{y} \delta(t_x, t_y) w(\vec{x}, \vec{y}) \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \right]_H \\ &= \hat{h}(1) \hat{\psi}_H(1) + \int_c d2 w(1, 2) \hat{\psi}_H^\dagger(2) \hat{\psi}_H(2) \hat{\psi}_H(1) \end{aligned} \quad (1.155)$$

(the time integration is considered on the contour) Analogously,

$$i\partial_{t_1} \hat{\psi}_H^\dagger(1) = -\hat{h}(1) \hat{\psi}_H^\dagger(1) - \int_c d2 w(1, 2) \hat{\psi}_H^\dagger(1) \hat{\psi}_H^\dagger(2) \hat{\psi}_H(2) \quad (1.156)$$

Now for the one-particle Green's function:

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

Concerning the first term

$$\delta(t_1, t_2) (\langle \hat{\psi}_H(1) \hat{\psi}_H^\dagger(2) \rangle + \langle \hat{\psi}_H^\dagger(2) \hat{\psi}_H(1) \rangle) = \delta(1, 2) \quad (1.157)$$

And in the remaining part, equation 1.155 will be used to obtain:

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

and further, by writing $1^+ = x_1, t_1 + \delta$ where $\delta \rightarrow 0$:

$$(i\partial_{t_1} - \hat{h}(1))G(1, 2) = \delta(1, 2) - i \int_c d3w(1^+, 3) \langle T_c[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)] \rangle \quad (1.158)$$

The average of the contour-ordered product of the four field operators in the r.h.s. of equation 1.158 is similar to a quantity that can be defined as a two-particle Green's function:

$$G_2(1, 2, 1', 2') = -\langle T_c[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}_H^\dagger(1')\hat{\psi}_H^\dagger(2')] \rangle \quad (1.159)$$

Thus:

$$(i\partial_{t_1} - \hat{h}(1))G(1, 2) = \delta(1, 2) - i \int_c d3w(1^+, 3)G_2(1, 3, 3^+, 2) \quad (1.160)$$

$$(-i\partial_{t_2} - \hat{h}(2))G(1, 2) = \delta(1, 2) - i \int_c d3w(2^+, 3)G_2(1, 3, 3^+, 2) \quad (1.161)$$

The purpose is to obtain self-consistent equations of motion for the Green's function, therefore the self-energy Σ will be defined so that the $-iG_2w$ term is replaced with a ΣG term which is a functional of G :

$$\int d2\Sigma(1, 2)G(2, 1') = -i \int_c d2w(1, 2)G_2(1, 2, 2^+, 1') \quad (1.162)$$

Then, the equations of motion can be written in the following way:

$$(i\partial_{t_1} - \hat{h}(1))G(1, 2) = \delta(1, 2) + \int_c d3\Sigma(1, 3)G(3, 2) \quad (1.163)$$

$$(-i\partial_{t_2} - \hat{h}(2))G(1, 2) = \delta(1, 2) + \int_c d3G(1, 3)\Sigma(3, 2) \quad (1.164)$$

Now, the requirement is to obtain the expression of Σ as a functional of G . To this end, consider a perturbation $\delta\hat{V}(t)$ in the Hamiltonian:

$$\delta\hat{V}(t) = \int d\vec{x}\delta v(\vec{x}t)\hat{n}(\vec{x}) \quad (1.165)$$

The change in the one-particle Green's function caused by this perturbation can be calculated by deriving the change in the time evolution operator from its equations of motion: (for a detailed derivation of the following formula, see Appendix A.9)

$$\frac{\delta G(1, 2)}{\delta v(3)} = -\langle T_c[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\hat{n}_H(3)] \rangle + \langle \hat{n}_H(3) \rangle \langle T_c[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)] \rangle \quad (1.166)$$

The first term in the r.h.s. is the two-particle Green's function and is useful to replace in equations 1.160, 1.161 to yield:

$$\begin{aligned} (i\partial_{t_1} - \hat{h}(1))G(1, 1') &= \delta(1, 1') + i \int_c d2w(1^+, 2) \frac{\delta G(1, 1')}{\delta v(2)} \\ &\quad + G(1, 1') \int_c d2w(1, 2) \langle \hat{n}_H(2) \rangle \end{aligned} \quad (1.167)$$

$$\begin{aligned} (-i\partial_{t_{1'}} - \hat{h}(1'))G(1, 1') &= \delta(1, 1') + i \int_c d2w(1^{++}, 2) \frac{\delta G(1, 1')}{\delta v(2)} \\ &\quad + G(1, 1') \int_c d2w(1', 2) \langle \hat{n}_H(2) \rangle \end{aligned} \quad (1.168)$$

A reasonable step to make next would be to connect the quantity $\frac{\delta G(1, 1')}{\delta v(2)}$ to Σ . To achieve this, one can differentiate equations 1.163, 1.164 with respect to the perturbation v :

$$\begin{aligned} (i\partial_{t_1} - \hat{h}(1))\frac{\delta G(1, 1')}{\delta v(2)} &= \delta(1, 2)G(1, 1') + \int_c d3 \frac{\delta \Sigma(1, 3)}{\delta v(2)} G(3, 1') \\ &\quad + \int_c d3\Sigma(1, 3) \frac{\delta G(3, 1')}{\delta v(2)} \end{aligned} \quad (1.169)$$

$$\begin{aligned}
(-i\partial_{t_1'} - \hat{h}(1'))\frac{\delta G(1, 1')}{\delta v(2)} &= \delta(1', 2)G(1, 1') + \int_c d3 \frac{\delta \Sigma(3, 1')}{\delta v(2)} G(1, 3) \\
&+ \int d3 \Sigma(3, 1') \frac{\delta G(1, 3)}{\delta v(2)}
\end{aligned} \tag{1.170}$$

The solution to these equations, after employing proper boundary conditions is:[1]

$$\frac{\delta G(1, 1')}{\delta v(2)} = G(1, 2)G(2, 1') + \int_c d3 d4 G(1, 3) \frac{\delta \Sigma(3, 4)}{\delta v(2)} G(4, 1') \tag{1.171}$$

(the derivation of boundary conditions and more details on this equation can be seen in Appendix A.10)
For simplicity in writing down the equations, define the vertex function Γ as:

$$\Gamma(12; 3) = \delta(1, 2)\delta(2, 3) + \frac{\delta \Sigma(1, 2)}{\delta v(3)} \tag{1.172}$$

Now,

$$\frac{\delta G(1, 1')}{\delta v(2)} = \int_c d3 d4 G(1, 3)G(4, 1')\Gamma(34; 2) \tag{1.173}$$

Replacing this into equations 1.167, 1.168 gives rise to the desired result, a self consistent equation for Σ which can be used iteratively to generate expressions for Σ as a functional of the one-particle Green's function:

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

Then:

$$\begin{aligned}
\Sigma(1, 2) &= i \int_c d3 d4 G(1, 3)w(1^+, 4)\Gamma(32; 4) - i\delta(1, 2) \int_c d3 w(1, 3)G(3, 3^+) \\
&= iG(1, 2)w(1^+, 2) - i\delta(1, 2) \int_c d3 w(1, 3)G(3, 3^+) \\
&+ i \int_c d3 d4 G(1, 3)w(1^+, 4) \frac{\delta \Sigma(3, 2)}{\delta v(4)}
\end{aligned}$$

In:

$$\begin{aligned}
\Sigma(1, 2) &= iG(1, 2)w(1^+, 2) - i\delta(1, 2) \int_c d3 w(1, 3)G(3, 3^+) \\
&+ i \int_c d3 d4 G(1, 3)w(1^+, 4) \frac{\delta \Sigma(3, 2)}{\delta v(4)}
\end{aligned} \tag{1.174}$$

assigning to w a wiggly line and to G a solid line, the diagrammatic expression for the self-energy used in the previous subchapters is reborn.

Now, that a perturbation expansion for Σ can be written down, the one-particle Green's function can be computed by performing the contour integrals in equations 1.163, 1.164.

Mathematical tools and methods related to Keldysh formalism can be applied to these expressions yielding the Kadanoff-Baym equations:

$$(i\partial_{t_1} - \hat{h}(1))G^{\lessdot}(1, 2) = (\Sigma^R \cdot G^{\lessdot} + \Sigma^{\lessdot} \cdot G^A + \Sigma^{\lrcorner} \star G^{\lrcorner})(1, 2) \tag{1.175}$$

$$(-i\partial_{t_2} - \hat{h}(2))G^{\lessdot}(1, 2) = (\Sigma^{\lessdot} \cdot G^R + \Sigma^A \cdot G^{\lessdot} + \Sigma^{\lrcorner} \star G^{\lrcorner})(1, 2) \tag{1.176}$$

$$(i\partial_{t_1} - \hat{h}(1))G^{\lrcorner}(1, 2) = (\Sigma^R \cdot G^{\lrcorner} + \Sigma^{\lrcorner} \star G^M)(1, 2) \tag{1.177}$$

$$(-i\partial_{t_2} - \hat{h}(2))G^\Gamma(1, 2) = (\Sigma^A \cdot G^\Gamma + \Sigma^\Gamma \star G^M)(1, 2) \quad (1.178)$$

$$(i\partial_{\tau_1} - \hat{h}(1))G^M(1, 2) = i\delta(\tau_1 - \tau_2) + (\Sigma^M \star G^M)(1, 2) \quad (1.179)$$

$$(-i\partial_{\tau_2} - \hat{h}(2))G^M(1, 2) = i\delta(\tau_1 - \tau_2) + (\Sigma^M \star G^M)(1, 2) \quad (1.180)$$

(For the detailed derivation of these expressions, the definitions of the quantities involved in them and a presentation of the Keldysh book-keeping methods used, see Appendix A.11)

Solving the Kadanoff-Baym equations is therefore a very important goal in many-body perturbation theory. The algorithm used in practice to solve these equations and the approximations for Σ will be further discussed in the following chapters along with examples of numerical calculations.

2 Linear Response Theory

Introduction

In this chapter, many-body perturbation theory methods will be used to investigate the linear response of a discrete system of N sites which can be occupied by electrons according to Pauli's exclusion principle, to an external perturbation. Although the self-energy functional will be approximated to a restricted series of Feynman diagrams, the density response function will still obey the frequency sum-rule, a fundamental relation in linear response theory based on the gauge properties of the system.

2.1 General theory of linear response to an external perturbation for Hubbard chains

Consider a Hubbard chain, a system of N sites which can be occupied by electrons according to Pauli's exclusion principle. This model is frequently used in condensed matter physics to study conductivity related properties and low temperature phenomena. To describe this particular type of systems, a more appropriate representation of the Hamiltonian is required.

Let $\phi_i(\vec{x})$ be a complete set of orthonormal orbitals in a one-particle Hilbert space:

$$\delta_{ij} = \int d\vec{x} \phi_i^*(\vec{x}) \phi_j(\vec{x}) \quad (2.1)$$

$$\delta(\vec{x} - \vec{y}) = \sum_{i=1}^{\infty} \phi_i^*(\vec{x}) \phi_i(\vec{y}) \quad (2.2)$$

Define annihilation and creation operators with respect to this basis:

$$\hat{a}_i \equiv \int d\vec{x} \phi_i^*(\vec{x}) \hat{\psi}(\vec{x}) \quad (2.3)$$

$$\hat{a}_i^\dagger \equiv \int d\vec{x} \phi_i(\vec{x}) \hat{\psi}^\dagger(\vec{x}) \quad (2.4)$$

Anticommutation relations follow:

$$\delta_{ij} = \{\hat{a}_i^\dagger, \hat{a}_j\} \quad (2.5)$$

$$0 = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = \{\hat{a}_i, \hat{a}_j\} \quad (2.6)$$

In terms of these operators, the Hamiltonian in equation 1.140 can be written in the following form:

$$\hat{H}(t) = \sum_{ij} h_{ij}(t) \hat{a}_i^\dagger \hat{a}_j + \sum_{ijkl} v_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \quad (2.7)$$

where:

$$h_{ij}(t) = \int d\vec{x} \phi_i^*(\vec{x}) \hat{h}(\vec{x}, t) \phi_j(\vec{x}) \quad (2.8)$$

$$v_{ijkl} = \frac{1}{2} \int d\vec{x} d\vec{y} \phi_i^*(\vec{x}) \phi_j^*(\vec{y}) w(\vec{x}, \vec{y}) \phi_k(\vec{y}) \phi_l(\vec{x}) \quad (2.9)$$

In the system of sites case, the orthonormal basis state vectors ϕ_i can be chosen to be spatial functions. $|\phi_i(\vec{x})|^2$ represents the probability of finding the particle at site i . These orbitals are highly localized, therefore it would be a good approximation to assume:

$$v_{ijkl} \cong \delta_{il}\delta_{jk}v_{ij} \quad (2.10)$$

with:

$$v_{ij} = \int d\vec{x}d\vec{y} |\phi_i(\vec{x})|^2 w(\vec{x}, \vec{y}) |\phi_j(\vec{y})|^2 \quad (2.11)$$

Then, the Hamiltonian to be used is:

$$\hat{H}(t) = \sum_{ij} h_{ij}(t) \hat{a}_i^\dagger \hat{a}_j + \sum_{ij} v_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_i \quad (2.12)$$

The purpose of this section is to study the reaction of such a system to an external time-dependent perturbation.

A completely determined system with a time-independent Hamiltonian \hat{H}_0 (h_{ij} does not depend on time) is perturbed at $t = t_0$ by turning on an additional time-dependent Hamiltonian $\hat{H}^{ex}(t)$.

$$\hat{H}(t) = \hat{H}_0 + \hat{H}^{ex}(t) \quad (2.13)$$

In the interaction picture:

$$i\partial_t |\Psi_I\rangle = \hat{H}_I^{ex}(t) |\Psi_I\rangle \quad (2.14)$$

where:

$$|\Psi_I\rangle = e^{i\hat{H}_0 t} |\Psi\rangle \quad (2.15)$$

$$\hat{H}_I^{ex}(t) = e^{i\hat{H}_0 t} \hat{H}^{ex}(t) e^{-i\hat{H}_0 t} \quad (2.16)$$

Integrating equation 2.14 yields to first order the formal solution:[13]

$$\begin{aligned} |\Psi_I\rangle(t) &= |\Psi_I\rangle(t_0) - i \int_{t_0}^t dt' \hat{H}_I^{ex}(t') |\Psi_I\rangle(t') \\ &= |\Psi_I\rangle(t_0) - i \int_{t_0}^t dt' \hat{H}_I^{ex}(t') |\Psi_I\rangle(t_0) + \dots \end{aligned}$$

Then, the change in the expectation value of an operator \hat{A} due to the perturbation $\hat{H}^{ex}(t)$, to first order, is:

$$\delta\langle \hat{A}(t) \rangle = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle - \langle \Psi(t_0) | \hat{A} | \Psi(t_0) \rangle \quad (2.17)$$

$$= -i \int_{t_0}^t dt' \langle \Psi(t_0) | \left[\hat{A}_{\hat{H}_0}(t), \hat{H}_I^{ex}(t') \right] | \Psi(t_0) \rangle \quad (2.18)$$

with:

$$\hat{A}_{\hat{H}_0}(t) = e^{i\hat{H}_0 t} \hat{A} e^{-i\hat{H}_0 t} \quad (2.19)$$

If one choses the operator in question to be the probability density at site i and the perturbation to be of the form:

$$\hat{H}^{ex}(t) = \hat{n}_j v_j(t) \quad (2.20)$$

then equation 2.18 turns into:

$$\delta n_i(t) = \int_0^\infty \chi_{ij}^R(t-t') v_j(t') dt' \quad (2.21)$$

where:

$$\chi_{ij}^R(t-t') = -i\theta(t-t') \langle \left[\hat{n}_{\hat{H}_0}(i, t), \hat{n}_{\hat{H}_0}(j, t') \right] \rangle \quad (2.22)$$

The function χ_{ij}^R is called the retarded response function and relates first order changes in the density to first order changes in the potential.

If

$$v_j(t) = \delta(t) \quad (2.23)$$

then

$$\delta n_i(t) = \chi_{ij}^R(t) \quad (2.24)$$

and in the limit $t \rightarrow 0^+$:

$$\partial_t n_i(0^+) = \lim_{t \rightarrow 0^+} \partial_t \chi_{ij}^R(t) \quad (2.25)$$

$$= -i \lim_{t \rightarrow 0^+} \langle [\partial_t \hat{n}_{\hat{H}_0}(i, t), \hat{n}_{\hat{H}_0}(j, 0)] \rangle \quad (2.26)$$

$$= -\langle [[\hat{n}_{\hat{H}_0}(i, 0), \hat{H}_0], \hat{n}_{\hat{H}_0}(j, 0)] \rangle \quad (2.27)$$

In conclusion,

$$\partial_t \chi_{ij}^R(0^+) = -\langle [[\hat{n}_i, \hat{H}_0], \hat{n}_j] \rangle \quad (2.28)$$

Calculating the commutators explicitly for:

$$\hat{H}_0 = \sum_{ij} h_{ij}(t) \hat{a}_i^\dagger \hat{a}_j + \sum_{ij} v_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_i \quad (2.29)$$

and

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \quad (2.30)$$

yields:

$$-\partial_t \chi_{ij}^R(0^+) = h_{ij} \gamma_{ji} + h_{ji} \gamma_{ij} - \delta_{ij} \sum_k (h_{ik} \gamma_{ki} + \gamma_{ik} h_{ki}) \quad (2.31)$$

where:

$$\gamma_{ij} = \langle \hat{a}_j^\dagger \hat{a}_i \rangle \quad (2.32)$$

Equation 2.31 is essentially the so-called frequency sum-rule. It will be shown that this relation also holds for the same quantities calculated within specific approximations with the Green's functions formalism.

But first, it is interesting to study more properties of the response function calculated with exact methods.

From the definition of χ , by inserting the complete set of eigenstates representing the excitation spectrum of the non-interacting system, the following analysis of how this function behaves in frequency space can be performed:[13]

$$i\chi_{ij}^R(t-t') = \theta(t-t') (\langle \Psi_0 | \hat{n}_{\hat{H}_0}(i, t) \hat{n}_{\hat{H}_0}(j, t') - \hat{n}_{\hat{H}_0}(j, t') \hat{n}_{\hat{H}_0}(i, t) | \Psi_0 \rangle) \quad (2.33)$$

$$= \sum_s (e^{i(E_0 - E_{N,s})(t-t')} \langle \Psi_0 | \hat{n}_i | \Psi_0 \rangle \langle \Psi_0 | \hat{n}_j | \Psi_0 \rangle - (e^{i(E_0 - E_{N,s})(t-t')} \langle \Psi_0 | \hat{n}_j | \Psi_0 \rangle \langle \Psi_0 | \hat{n}_i | \Psi_0 \rangle)) \quad (2.34)$$

(It was used that: $\hat{H}_0 |N, s\rangle = E_{N,s} |N, s\rangle$) Therefore:

$$\chi_{ij}^R(t-t') = -i\theta(t-t') \sum_s e^{-i\Omega_{N,s}(t-t')} f_{N,s}(i) f_{N,s}^*(j) + c.c \quad (2.35)$$

where:

$$f_{N,s}(i) = \langle \Psi_0 | \hat{n}_i | N, s \rangle \quad (2.36)$$

$$\Omega_{N,s} = E_{N,s} - E_0 \quad (2.37)$$

Using the following representation of the step function:

$$\theta(\tau) = \lim_{\eta \rightarrow 0^+} -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{e^{i\omega\tau}}{\omega + i\eta} \quad (2.38)$$

the Fourier transform of equation 2.35 can be calculated to be:

$$\tilde{\chi}_{ij}^R(\omega) = \lim_{\eta \rightarrow 0^+} \sum_s \left(\frac{f_{N,s}(i)f_{N,s}^*(j)}{\omega - \Omega_{N,s} + i\eta} - \frac{f_{N,s}(i)f_{N,s}^*(j)}{\omega + \Omega_{N,s} + i\eta} \right) \quad (2.39)$$

This shows that $\tilde{\chi}_{ij}^R(\omega)$ has poles at $\omega = \pm\Omega_{N,s} - i\eta$

For a time reversal invariant system, the states $|N, s\rangle$ and $|\Psi_0\rangle$ can be chosen to be real. Then,

$$f_{N,s}(i) = f_{N,s}^*(i) \quad (2.40)$$

and:

$$\tilde{\chi}_{ij}^R(\omega) = \lim_{\eta \rightarrow 0^+} \sum_s f_{N,s}(i)f_{N,s}(j) \left(\frac{1}{\omega - \Omega_{N,s} + i\eta} - \frac{1}{\omega + \Omega_{N,s} + i\eta} \right) \quad (2.41)$$

Further, using a well-known formula in complex analysis:

$$\lim_{\eta \rightarrow 0} \frac{1}{\omega + i\eta} = P\left(\frac{1}{\omega}\right) - i\pi\delta(\omega) \quad (2.42)$$

leads to:

$$\Re\tilde{\chi}_{ij}^R(\omega) = \sum_s f_{N,s}(i)f_{N,s}(j)P\left(\frac{1}{\omega - \Omega_{N,s}} - \frac{1}{\omega + \Omega_{N,s}}\right) \quad (2.43)$$

and:

$$\Im\tilde{\chi}_{ij}^R(\omega) = -\pi \sum_s f_{N,s}(i)f_{N,s}(j) (\delta(\omega - \Omega_{N,s}) - \delta(\omega + \Omega_{N,s})) \quad (2.44)$$

Thus, by calculating the density response function, information on the optical spectrum of the system can be obtained.

Also, it will be interesting to investigate the peak structure of the response function calculated within approximations to see how close to its poles lie the exact excitation energies.

2.2 The frequency sum-rule in Green's functions formalism

The frequency sum-rule in Green's function's formalism can be deduced as a consequence of a Ward identity describing the gauge properties of the system. The following derivation summarizes the analysis made on this topic in reference [10]

Perform a gauge transformation:

$$\vec{A}(\vec{r}z) \rightarrow \vec{A}(\vec{r}z) + \nabla\Lambda(\vec{r}z) \quad (2.45)$$

$$v(\vec{r}z) \rightarrow v(\vec{r}z) - \frac{1}{c}\partial_z\Lambda(\vec{r}z) \quad (2.46)$$

to the electromagnetic field in the one-body part of the Hamiltonian:

$$h(\vec{r}z) = \frac{1}{2m} \left(-i\nabla - \frac{q}{c}\vec{A}(\vec{r}z) \right)^2 + qv(\vec{r}z) \quad (2.47)$$

(z is the time-contour variable). The new one-body matrix elements will be[10]:

$$h_{ij}^\Lambda(z) = \int d\vec{x}\phi_i^*(\vec{x}) \left(\frac{1}{2m} \left(-i\nabla - \frac{q}{c}(\vec{A}(\vec{r}z) + \nabla\Lambda) \right)^2 + qv - \frac{q}{c}\partial_z\Lambda \right) \phi_j(\vec{x}) \quad (2.48)$$

$$\begin{aligned} &= \int d\vec{x}\phi_i^*(\vec{x}) e^{i\frac{q}{c}\Lambda(\vec{r}z)} \left(\frac{1}{2m} \left(-i\nabla - \frac{q}{c}\vec{A}(\vec{r}z) \right)^2 + qv(\vec{r}z) - \frac{q}{c}\partial_z\Lambda \right) \\ &\times e^{-i\frac{q}{c}\Lambda(\vec{r}z)} \phi_j(\vec{x}) \end{aligned} \quad (2.49)$$

Since the orbitals are localized around lattice positions \vec{R}_j , it is a good approximation to write[10]:

$$e^{-i\frac{q}{c}\Lambda(\vec{r}z)} \phi_j(\vec{x}) = e^{-i\frac{q}{c}\Lambda(\vec{R}_jz)} \phi_j(\vec{x}) = e^{-i\frac{q}{c}\Lambda_j(z)} \phi_j(\vec{x}) \quad (2.50)$$

Then:

$$h_{ij}^\Lambda(z) = e^{i\frac{q}{c}\Lambda_i(z)} h_{ij}(z) e^{-i\frac{q}{c}\Lambda_j(z)} - \delta_{ij} \frac{q}{c} \partial_z \Lambda_i(z) \quad (2.51)$$

The two-body part of the Hamiltonian remains the same. Therefore, the gauge transformed Hamiltonian can be written as:

$$\begin{aligned} \hat{H}^\Lambda(z) &= \sum_{ij} \left(e^{i\frac{q}{c}(\Lambda_i - \Lambda_j)} h_{ij} - \delta_{ij} \frac{q}{c} \partial_z \Lambda_i \right) \hat{a}_i^\dagger \hat{a}_j \\ &+ \frac{1}{2} \sum_{ij} v_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_i \end{aligned} \quad (2.52)$$

If $G_{ij}(z, z')$ satisfies the Kadanoff-Baym equations for the Hamiltonian $\hat{H}(z)$ within an approximation for the self-energy which can be expressed diagrammatically:

$$(i\partial_z - \hat{h}(z))G(z, z') = \delta(z, z') + \int_c dz'' \Sigma[G](z, z'')G(z'', z') \quad (2.53)$$

then,

$$G_{ij}^\Lambda(z, z') = e^{i\frac{q}{c}\Lambda_i(z)} G_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z')} \quad (2.54)$$

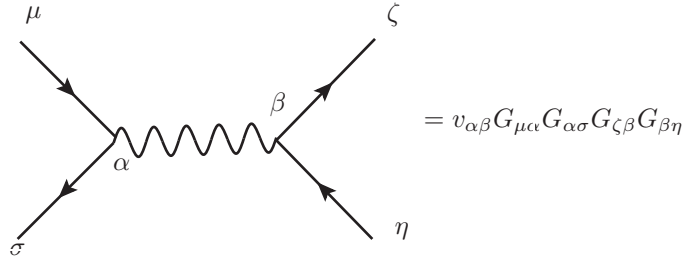
satisfies the Kadanoff-Baym equations for the Hamiltonian $\hat{H}^\Lambda(z)$ within the same approximation for Σ , i.e.:

$$(i\partial_z - \hat{h}^\Lambda(z))G^\Lambda(z, z') = \delta(z, z') + \int_c dz'' \Sigma^\Lambda[G^\Lambda](z, z'')G^\Lambda(z'', z') \quad (2.55)$$

The proof of this statement can be found in Reference [10] and can be summarized in the following way:

$$\begin{aligned} i\partial_z G_{ij}^\Lambda(z, z') &= -\frac{q}{c} (\partial_z \Lambda_i(z)) e^{i\frac{q}{c}\Lambda_i(z)} G_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z')} \\ &+ i e^{i\frac{q}{c}\Lambda_i(z)} \partial_z G_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z')} \\ &= -\frac{q}{c} (\partial_z \Lambda_i(z)) G_{ij}^\Lambda(z, z') + \delta_{ij} \delta(z, z') \\ &+ \sum_k e^{i\frac{q}{c}\Lambda_i(z)} h_{ik}(z) e^{-i\frac{q}{c}\Lambda_k(z)} e^{i\frac{q}{c}\Lambda_k(z)} G_{kj}(z, z') e^{-i\frac{q}{c}\Lambda_j(z)} \\ &+ e^{i\frac{q}{c}\Lambda_i(z)} \left(\int \Sigma[G]G \right)_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z)} \\ &= \sum_k h_{ik}^\Lambda G_{kj}^\Lambda(z, z') + e^{i\frac{q}{c}\Lambda_i(z)} \left(\int \Sigma[G]G \right)_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z)} \end{aligned}$$

In a Feynman diagram



replace all the G_{ij} with $e^{i\frac{q}{c}\Lambda_i(z)} G_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z)}$.

Then the value of the diagram will become $e^{i\frac{q}{c}(\Lambda_\mu - \Lambda_\sigma + \Lambda_\zeta - \Lambda_\eta)} v_{\alpha\beta} G_{\mu\alpha} G_{\alpha\sigma} G_{\zeta\beta} G_{\beta\eta}$. The phase factors corresponding to internal vertices cancel out. Also, in the self-energy diagrams $\zeta = \eta$ (there are only two lines connecting a self-energy insertion to the rest of the diagram) therefore:

$$e^{i\frac{q}{c}\Lambda_i(z)} \left(\int \Sigma[G]G \right)_{ij}(z, z') e^{-i\frac{q}{c}\Lambda_j(z)} = \left(\int \Sigma^\Lambda[G^\Lambda]G^\Lambda \right)_{ij}(z, z') \quad (2.56)$$

This concludes the proof.

From equation 2.54, to first order in Λ , the change in the Green's function is:

$$\delta G_{ij}^\Lambda(z, z') = i \frac{q}{c} (\Lambda_i(z) - \Lambda_j(z')) G_{ij}(z, z') \quad (2.57)$$

On the other hand, the Hamiltonian can also be expanded in terms of Λ :

$$\hat{H}^\Lambda(z) = \hat{H}_0^\Lambda(z) + \sum_{ij} f_{ij}(z) \hat{a}_i^\dagger \hat{a}_j + \mathcal{O}(\Lambda^2) \quad (2.58)$$

where:

$$f_{ij}(z) = \frac{q}{c} (i(\Lambda_i - \Lambda_j) h_{ij} - \delta_{ij} \partial_z \Lambda_i) \quad (2.59)$$

The last term in equation 2.59: $\sum_{ij} f_{ij} \hat{a}_i^\dagger \hat{a}_j$ can be regarded as an external perturbation to the initial Hamiltonian. The Green's function can also be expanded with respect to this general external perturbation (f_{ij} can take any form):

$$G_{ij}(z, z') = G_{ij}(z, z')|_{f_{ij}=0} + \sum_{kl} \int_c \frac{\delta G_{ij}(z, z')}{\delta f_{kl}(z'')} \Big|_{f_{kl}=0} f_{kl}(z'') dz'' + \dots \quad (2.60)$$

Therefore the first order change in the Green's function is:

$$\delta G_{ij}(z, z') = \sum_{kl} \int_c \frac{\delta G_{ij}(z, z')}{\delta f_{kl}(z'')} \Big|_{f_{kl}=0} f_{kl}(z'') dz'' \quad (2.61)$$

Defining:

$$\Gamma_{ij,kl}(z, z'; z'') = \frac{\delta G_{ij}(z, z')}{\delta f_{kl}(z'')} \Big|_{f_{kl}=0} \quad (2.62)$$

relation 2.61 becomes:

$$\begin{aligned} \delta G_{ij}(z, z') &= \sum_{kl} \int_c dz'' \Gamma_{ij,kl}(z, z'; z'') \frac{q}{c} (i(\Lambda_k - \Lambda_l) h_{kl} \\ &\quad - \delta_{kl} \partial_{z''} \Lambda_k) \end{aligned} \quad (2.63)$$

The next step is to integrate by parts assuming the boundary condition $\Lambda_k(t_0) = \Lambda_k(t_0 - i\beta)$ to yield:

$$\begin{aligned} \delta G_{ij}(z, z') &= i \frac{q}{c} \sum_{kl} \int_c dz'' \Gamma_{ij,kl}(z, z'; z'') (\Lambda_k(z'') - \Lambda_l(z'')) h_{kl}(z'') \\ &\quad + \delta_{kl} \int_c dz'' (\partial_{z''} \Gamma_{ij,kl}(z, z'; z'')) \Lambda_k(z'') \end{aligned}$$

Identifying this change in the Green's function with the change described by equation 2.57 implies:

$$\begin{aligned} i \frac{q}{c} \sum_k \int_c dz'' (\delta_{ik} \delta(z, z'') - \delta_{jk} \delta(z', z'')) G_{ij}(z, z') \Lambda_k(z'') = \\ i \sum_k \int_c dz'' \sum_l (\Gamma_{ij,kl}(z, z'; z'') h_{kl}(z'') - \Gamma_{ij,lk}(z, z'; z'') h_{lk}(z'')) \\ - i \delta_{kl} \partial_{z''} \Gamma_{ij,kl}(z, z'; z'') \Lambda_k(z'') \end{aligned}$$

Since this is true for any $\Lambda_k(z'')$, then:

$$\begin{aligned} (\delta_{ik} \delta(z, z'') - \delta_{jk} \delta(z', z'')) G_{ij}(z, z') &= \sum_l (\Gamma_{ij,kl}(z, z'; z'') \\ &\quad h_{kl}(z'') - \Gamma_{ij,lk}(z, z'; z'') h_{lk}(z'')) - i \partial_{z''} \Gamma_{ij,kl}(z, z'; z'') \end{aligned} \quad (2.64)$$

$$(2.65)$$

This last equation is a Ward identity[10]. If one takes the limit $z' \rightarrow z$ and if one defines the density matrix and the response function as:

$$\gamma_{ij}(z) = -iG_{ij}(z, z^+) \quad (2.66)$$

and:

$$\chi_{ij,lk}(z, z') = -i \left. \frac{\delta G_{ij}(z, z^+)}{\delta f_{kl}(z')} \right|_{f_{kl}=0} \quad (2.67)$$

then, the Ward identity for the response function will be:[10]

$$\begin{aligned} (\delta_{ik}\delta(z, z'') - \delta_{jk}\delta(z, z'')) \gamma_{ij}(z) &= \sum_l (\chi_{ij,lk}(z, z'')h_{kl}(z'') \\ &- \chi_{ij,kl}(z, z'')h_{lk}(z'')) - i\partial_{z''}\chi_{ij,kk}(z, z'') \end{aligned} \quad (2.68)$$

The response function belongs to the Keldysh space, i.e.

$$\chi_{ij,lk}(z, z') = \theta(z, z')\chi_{ij,lk}^>(z, z') + \theta(z', z)\chi_{ij,lk}^<(z, z') \quad (2.69)$$

Differentiating 2.69 with respect to z' yields:

$$\begin{aligned} \partial_{z'}\chi_{ij,lk}(z, z') &= -\delta(z, z') (\chi_{ij,lk}^>(z, z') - \chi_{ij,lk}^<(z, z')) \\ &+ \theta(z, z')\partial_{z'}\chi_{ij,lk}^>(z, z') + \theta(z', z)\partial_{z'}\chi_{ij,lk}^<(z, z') \end{aligned} \quad (2.70)$$

The insertion of 2.69 and 2.70 into the Ward identity, results in the following equalities:

$$i\partial_{z'}\chi_{ij,kk}^>(z, z') = \sum_l \chi_{ij,lk}^>(z, z')h_{kl}(z') - \chi_{ij,kl}^>(z, z')h_{lk}(z') \quad (2.71)$$

$$i\partial_{z'}\chi_{ij,kk}^<(z, z') = \sum_l \chi_{ij,lk}^<(z, z')h_{kl}(z') - \chi_{ij,kl}^<(z, z')h_{lk}(z') \quad (2.72)$$

and

$$i(\chi_{ij,kk}^>(z, z') - \chi_{ij,kk}^<(z, z')) = (\delta_{ik} - \delta_{jk})\gamma_{ij}(z) \quad (2.73)$$

Then,

$$\begin{aligned} i\partial_{z'}(\chi_{ij,kk}^> - \chi_{ij,kk}^<)(z, z') \Big|_{z=z'} &= \sum_l (\chi^> - \chi^<)_{ii,lk}(z, z)h_{kl}(z) \\ &- (\chi^> - \chi^<)_{ii,kl}(z, z)h_{lk}(z) \end{aligned} \quad (2.74)$$

When the Kadanoff-Baym equations are solved self-consistently, one cannot sum all the diagrams for the self energy. An approximation must be made. Since the expectation values of operators depend on the approximation for Σ , it is desired to make only such approximations that preserve the conservation laws of Nature. Gordon Baym proved that if one starts with an approximation for Σ as a functional of G and of the two particle interaction, such that Σ is of the form $\frac{\delta\Phi}{\delta G}$ where Φ is a "closed" functional of G , then the non-equilibrium function G obeys the differential number conservation law and the total momentum (angular momentum) and energy conservation laws.[11]

Using a conserving approximation for Σ results in a symmetry property for χ . Using a short notation, the derivation can proceed as follows:

$$\chi = -i \frac{\delta G}{\delta v} \quad (2.75)$$

Since

$$GG^{-1} = 1 \quad (2.76)$$

then

$$\frac{\delta G}{\delta v}G^{-1} + G\frac{\delta G^{-1}}{\delta v} = 0 \quad (2.77)$$

and

$$\frac{\delta G}{\delta v} = -G \frac{\delta G^{-1}}{\delta v} G \quad (2.78)$$

From the equation of motion for the Green's function:

$$(i\partial_t - h_0 - v)G - \Sigma G = 1 \quad (2.79)$$

it can be implied that:

$$G^{-1} = i\partial_t - h_0 - v - \Sigma \quad (2.80)$$

Then:

$$\frac{\delta G^{-1}}{\delta v} = -1 - \frac{\delta \Sigma}{\delta v} \quad (2.81)$$

Replacing this in equation 2.77 results in:

$$\chi = -i(GG + G \frac{\delta \Sigma}{\delta v} G) \quad (2.82)$$

Using the chain rule:

$$\frac{\delta \Sigma}{\delta v} = \frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta v} \quad (2.83)$$

one can obtain:

$$\chi = -i \left(GG + iG \frac{\delta \Sigma}{\delta G} \chi G \right) \quad (2.84)$$

and further:

$$\left(G^{-1}G^{-1} - \frac{\delta \Sigma}{\delta G} \right) \chi = 1 \quad (2.85)$$

or:

$$G^{-1}G^{-1} - \frac{\delta \Sigma}{\delta G} = \chi^{-1} \quad (2.86)$$

More explicitly,

$$G^{-1}(1, 2)G^{-1}(2, 1^+) - \frac{\delta \Sigma(1, 1^+)}{\delta G(2, 2^+)} = \chi^{-1}(1, 2) \quad (2.87)$$

The l.h.s. of equation 2.87 is symmetric under the interchange of indices 1 and 2 for conserving approximations:

$$\frac{\delta \Sigma(1, 1^+)}{\delta G(2, 2^+)} = \frac{\delta^2 \Phi}{\delta G(1, 1^+) \delta G(2, 2^+)} = \frac{\delta \Sigma(2, 2^+)}{\delta G(1, 1^+)} \quad (2.88)$$

Therefore χ^{-1} and also χ have this symmetry property. For the Hubbard system:

$$\chi_{ij, lk}(z, z') = \chi_{lk, ij}(z', z) \quad (2.89)$$

which implies:

$$\chi_{ij, lk}^>(z, z') = \chi_{lk, ij}^<(z', z) \quad (2.90)$$

Using this symmetry property in equation 2.74, it can be obtained that:

$$\begin{aligned} i\partial_{z'}(\chi_{ii, kk}^> - \chi_{ii, kk}^<)(z, z') \Big|_{z=z'} &= -\sum_l (\chi^> - \chi^<)_{lk, ii}(z, z) h_{kl}(z) \\ +(\chi^> - \chi^<)_{kl, ii}(z, z) h_{lk}(z) &= i \sum_l ((\delta_{li} - \delta_{ki}) \gamma_{lk}(z) h_{kl}(z) \\ -(\delta_{ki} - \delta_{li}) \gamma_{kl}(z) h_{lk}(z)) &= i(\gamma_{ik}(z) h_{ki}(z) + \gamma_{ki}(z) h_{ik}(z)) \\ -\sum_l \delta_{ki} (\gamma_{lk}(z) h_{kl}(z) - \gamma_{kl}(z) h_{lk}(z)) & \end{aligned} \quad (2.91)$$

As in the exact treatment, the aim is to study the response of a system which was initially in equilibrium (h_{ij} time-independent) to an external perturbation. In that case, for a homogeneous system, the Green's functions and the response functions also, depend on the difference of the time arguments. Also, in

order to compare to the exact calculation discussed in the previous subsection, zero-temperature will be assumed.

Thus:

$$\partial_{t'}(\chi_{ik}^> - \chi_{ik}^<)(t - t')|_{t=t'} = -\partial_{\tau}(\chi_{ik}^> - \chi_{ik}^<)(\tau)|_{\tau=0} \quad (2.92)$$

(where the short notation $\chi_{ik} \equiv \chi_{ii,kk}$ was used)

The retarded response function in the τ variable is:

$$\chi_{ij}^R(\tau) = \theta(\tau)(\chi_{ij}^>(\tau) - \chi_{ij}^<(\tau)) \quad (2.93)$$

Derivating with respect to τ equation 2.93:

$$\partial_{\tau}\chi_{ij}^R(\tau) = \delta_{\tau}(\chi_{ij}^>(\tau) - \chi_{ij}^<(\tau)) + \theta(\tau)\partial_{\tau}(\chi_{ij}^>(\tau) - \chi_{ij}^<(\tau)) \quad (2.94)$$

and taking the limit $\tau \rightarrow 0^+$ yields:

$$\partial_{\tau}(\chi_{ij}^>(\tau) - \chi_{ij}^<(\tau))|_{\tau \rightarrow 0^+} = \partial_{\tau}\chi_{ij}^R(0^+) \quad (2.95)$$

Equation 2.95 is to be replaced in the calculation in 2.91 to reach the frequency sum-rule:

$$-\partial_{\tau}\chi_{ij}^R(0^+) = \gamma_{ik}(0^+)h_{ki} + \gamma_{ki}(0^+)h_{ik} - \delta_{ik} \sum_l (\gamma_{lk}(0^+)h_{kl} + \gamma_{kl}(0^+)h_{lk}) \quad (2.96)$$

This is the same frequency sum-rule that was written for the exact case in the previous subsection (equation 2.31) with the sole difference that the quantities χ and γ are now calculated by solving self-consistently the Kadanoff-Baym equations within a conserving approximation for Σ . [10] The Fourier transform of $\chi_{ij}^R(\tau)$ is:

$$\chi_{ij}^R(\omega) = \int_{-\infty}^{\infty} d\tau \theta(\tau) \bar{\chi}_{ij}(\tau) e^{i\omega\tau} \quad (2.97)$$

with:

$$\bar{\chi}_{ij}(\tau) = \chi_{ij}^>(\tau) - \chi_{ij}^<(\tau) \quad (2.98)$$

The representation for θ in equation 2.38 is to be used here too:

$$\begin{aligned} \chi_{ij}^R(\omega) &= \lim_{\eta \rightarrow 0^+} i \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \int_{-\infty}^{\infty} d\tau \frac{e^{i(\omega-\nu)\tau}}{\nu + i\eta} \bar{\chi}_{ij}(\tau) \\ &= \lim_{\eta \rightarrow 0^+} i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} d\tau \frac{e^{i\omega'\tau}}{\omega - \omega' + i\eta} \bar{\chi}_{ij}(\tau) \\ &= \lim_{\eta \rightarrow 0^+} i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\bar{\chi}_{ij}(\omega')}{\omega - \omega' + i\eta} \end{aligned} \quad (2.99)$$

From this calculation it can be concluded that $\chi_{ij}^R(\omega)$ has a pole structure. One cannot derive a Lehman representation for χ calculated within approximation schemes, however one may argue that since for a conserving approximation χ tends towards a close replica of the exact object, then the pole structure of χ also tends towards the case when the peaks correspond to the eigenenergies of the unperturbed system. In the next chapter, numerical illustrations will be presented to appreciate how well the response function calculated within some conserving approximations resembles the exact response function.

2.3 Diagrammatic analysis of the density response function

In this subchapter, a few of the simplest conserving approximations for Σ used in numerical calculations will be described diagrammatically along with the density response function corresponding to the approximation in question. This analysis follows reference [12].

The expectation value of the probability density at spacetime point 1 is:

$$n(1) = -iG(1, 1^+) \quad (2.100)$$

and the density response function was defined to be:

$$\chi(1, 2) = -i \frac{\delta G(1, 1^+)}{\delta v(2)} = \frac{\delta n(1)}{\delta v(2)} \quad (2.101)$$

where v is a perturbing potential.

The effective potential is defined as:

$$\phi(1) = v(1) + \int d2 w(1, 2) n(2) \quad (2.102)$$

($w(1, 2)$ is the two-body interaction).

Using the chain rule:

$$\chi(1, 2) = -i \int d3 \frac{\delta G(1, 1^+)}{\delta \phi(3)} \frac{\delta \phi(3)}{\delta v(2)} \quad (2.103)$$

$$= -i \int d3 \frac{\delta G(1, 1^+)}{\delta \phi(3)} \left(\delta(3, 2) + \int d4 w(3, 4) \frac{\delta n(4)}{\delta v(2)} \right) \quad (2.104)$$

$$= -i \frac{\delta G(1, 1^+)}{\delta \phi(2)} - i \int d3 d4 \frac{\delta G(1, 1^+)}{\delta \phi(3)} w(3, 4) \chi(4, 2) \quad (2.105)$$

and denoting the irreducible polarizability by:

$$P(1, 2) = \frac{\delta n(1)}{\delta \phi(2)} = -i \frac{\delta G(1, 1^+)}{\delta \phi(2)} \quad (2.106)$$

results in the following relation for χ : [12]

$$\chi(1, 2) = P(1, 2) + \int d3 d4 P(1, 3) w(3, 4) \chi(4, 2) \quad (2.107)$$

Diagrammatically, this relation can be represented as:



A more explicit expression for P is necessary.

The inverse Green's function satisfies the relation:

$$\int d2 G(1, 2) G^{-1}(2, 3) = \delta(1, 3) \quad (2.108)$$

Derivating with respect to the effective potential yields:

$$0 = \int d2 \left(\frac{\delta G(1, 2)}{\delta \phi(4)} G^{-1}(2, 3) + G(1, 2) \frac{\delta G^{-1}(2, 3)}{\delta \phi(4)} \right) \quad (2.109)$$

and further:

$$\int d2 d3 \frac{\delta G(1, 2)}{\delta \phi(4)} G^{-1}(2, 3) G(3, 5) = - \int d2 d3 G(1, 2) \frac{\delta G^{-1}(2, 3)}{\delta \phi(4)} G(3, 5) \quad (2.110)$$

which means:

$$\frac{\delta G(1, 5)}{\delta \phi(4)} = - \int d2 d3 G(1, 2) \frac{\delta G^{-1}(2, 3)}{\delta \phi(4)} G(3, 5) \quad (2.111)$$

and:

$$P(1, 2) = -i \frac{\delta G(1, 1^+)}{\delta \phi(2)} = -i \int d3 d4 G(1, 3) \frac{\delta G^{-1}(3, 4)}{\delta \phi(2)} G(4, 1^+) \quad (2.112)$$

From the equation of motion for the Green's function:

$$(i\partial_{t_1} - h_0(1) - v(1))G(1, 2) - \int d^3\Sigma(1, 3)G(3, 2) = \delta(1, 2) \quad (2.113)$$

rewritten as:

$$\int d^3\Sigma(\delta(3, 1)(i\partial_{t_1} - h_0(1) - v(1)) - \Sigma(1, 3))G(3, 2) = \delta(1, 2) \quad (2.114)$$

by comparison with 2.108 it can be seen that:

$$G^{-1}(1, 2) = \delta(1, 2)(i\partial_{t_1} - h_0(1) - v(1)) - \Sigma(1, 2) \quad (2.115)$$

If the tadpole diagram is separated from the self-energy:

$$\Sigma(1, 2) = \delta(1, 2) \int d^3w(1, 3)n(3) + \Sigma_{XC}(1, 2) \quad (2.116)$$

then

$$G^{-1}(1, 2) = \delta(1, 2)(i\partial_{t_1} - h_0(1) - \phi(1)) - \Sigma_{XC}(1, 2) \quad (2.117)$$

Defining the vertex function Γ as:[12]

$$\Gamma(12; 3) = -\frac{\delta G^{-1}(1, 2)}{\delta\phi(3)} \quad (2.118)$$

and using equation 2.117 yields:

$$\Gamma(12; 3) = \delta(1, 3)\delta(1, 2) + \frac{\delta\Sigma_{XC}(1, 2)}{\delta\phi(3)} \quad (2.119)$$

$$= \delta(1, 3)\delta(1, 2) + \int d^4d^5 \frac{\delta\Sigma_{XC}(1, 2)}{\delta G(4, 5)} \frac{\delta G(4, 5)}{\delta\phi(3)} \quad (2.120)$$

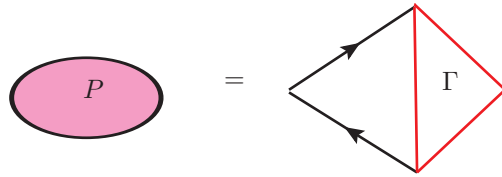
Taking into account equation 2.111 results in:

$$\Gamma(12; 3) = \delta(1, 3)\delta(1, 2) + \int d^4d^5d^6d^7 \frac{\delta\Sigma_{XC}(1, 2)}{\delta G(4, 5)} G(4, 6)\Gamma(67; 3)G(7, 5) \quad (2.121)$$

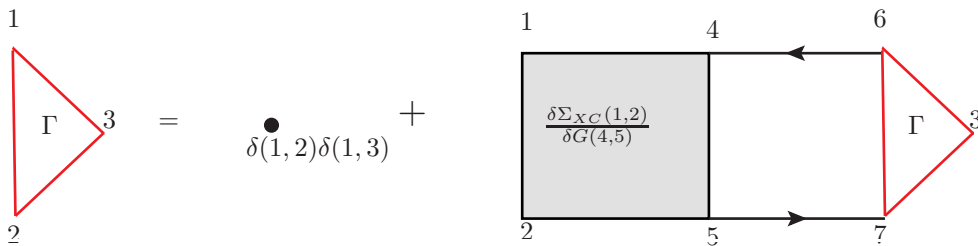
Equation 2.112 written in terms of the vertex function:

$$P(1, 2) = \int d^3d^4 G(1, 3)\Gamma(34; 2)G(4, 1^+) \quad (2.122)$$

and equation 2.121 can be expressed diagrammatically as:



and



The first conserving approximation to be discussed is the Hartree-Fock approximation:

$$\Sigma_{XC}^{HF}(1,2) = \text{Diagram 1}$$

$$\Phi^{HF} = \text{Diagram 2} + \text{Diagram 3}$$

$$\Sigma^{HF} = \frac{\delta\Phi^{HF}}{\delta G} = \text{Diagram 4} + \text{Diagram 5}$$

When using this approximation one assumes that each particle moves in a single particle potential that comes from its average interaction with all the other particles. Even though only the first order in the interaction w digrams contributing to Σ are retained, this approximation will result in a third order approximation for the density response function:

$$\frac{\delta\Sigma_{XC}^{HF}}{\delta G} = \text{Diagram 6}$$

$$\Gamma = \text{Diagram 7} + \text{Diagram 8}$$

$$= \text{Diagram 9} + \text{Diagram 10} + \text{Diagram 11} + \dots$$

$$P = \text{Diagram 12} + \text{Diagram 13} + \dots$$

$$\chi = \text{Diagram 14} + \text{Diagram 15} + \dots$$

$$+ \text{Diagram 16} + \text{Diagram 17} + \dots$$

If the second order skeleton diagrams are added, the second Born approximation is obtained:

$$\Sigma_{XC}^{2B} = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]}$$

$$\frac{\Sigma_{XC}^{2B}}{\delta G} = \text{[diagram 4]} + \text{[diagram 5]} + \text{[diagram 6]} + \text{[diagram 7]}$$

$$+ \text{[diagram 8]} + \text{[diagram 9]} + \text{[diagram 10]}$$

These diagrams will result in a complex, fifth order in w structure for χ .

The final approximation that will be used in the numerical examples in this thesis is called the GW approximation. To understand this approximation, some further diagrammatic analysis is necessary:

A diagram is called a polarization insertion if it can be cut from a diagram by cutting two interaction lines[7]:



Define the dynamically screened interaction W as:

$$W = \text{[wavy line]} = \text{[wavy line]} + \text{[wavy line with } \bar{P} \text{]} + \text{[wavy line with } \bar{P} \text{ and } \bar{P} \text{]} + \dots$$

where \bar{P} is the sum of all possible irreducible polarization insertions (the diagrams in \bar{P} cannot be cut in two by cutting a single interaction line).

$$\bar{P} = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

Σ_{XC} can now be expressed in terms of the dynamically screened interaction by considering all diagrams which have no polarization insertions and replace w with W .

$$\Sigma_{XC}[G, W] = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

Approximating by keeping only the first term in this expansion and the first order in w term in the expansion of \bar{P} results in the so-called GW approximation. It is also a conserving approximation:[1]

$$\begin{aligned} \Phi^{GW} &= -\frac{1}{2} \text{[diagram: circle with wavy line]} - \frac{1}{4} \text{[diagram: two circles with wavy line]} - \frac{1}{6} \text{[diagram: three circles with wavy line]} + \dots \\ \Sigma^{GW} &= \text{[diagram: wavy line]} + \text{[diagram: circle with wavy line]} + \text{[diagram: two circles with wavy line]} + \dots \end{aligned}$$

$$\frac{\delta \Sigma_{XC}(1, 2)}{\delta G(4, 5)} = i\delta(1, 4)\delta(2, 5)W(1, 2) + iG(1, 2)\frac{\delta W(1, 2)}{\delta G(4, 5)} \quad (2.123)$$

$$W(1, 2) = w(1, 2) + \int d3d4w(1, 3)\bar{P}(3, 4)W(4, 3) \quad (2.124)$$

Introducing the inverse of the screened interaction:

$$\int d2W(1, 2)W^{-1}(2, 3) = \delta(1, 3) = \int d2w(1, 2)W^{-1}(2, 3) + \int d5w(1, 5)\bar{P}(5, 3) \quad (2.125)$$

allows one to write:[12]

$$w^{-1} = W^{-1} + \bar{P} \quad (2.126)$$

On the other hand:

$$\frac{\delta W(1, 2)}{\delta G(4, 5)} = - \int d6d7W(1, 6)\frac{\delta W^{-1}(6, 7)}{\delta G(4, 5)}W(7, 2) \quad (2.127)$$

Thus:

$$\frac{\delta W(1, 2)}{\delta G(4, 5)} = \int d6d7W(1, 6)\frac{\delta \bar{P}(6, 7)}{\delta G(4, 5)}W(7, 2) \quad (2.128)$$

Since

$$\bar{P}(1, 2) = G(1, 2)G(2, 1) \quad (2.129)$$

then

$$\frac{\delta W(1, 2)}{\delta G(4, 5)} = -iW(1, 4)G(5, 4)W(5, 2) - iW(1, 5)G(5, 4)W(4, 2) \quad (2.130)$$

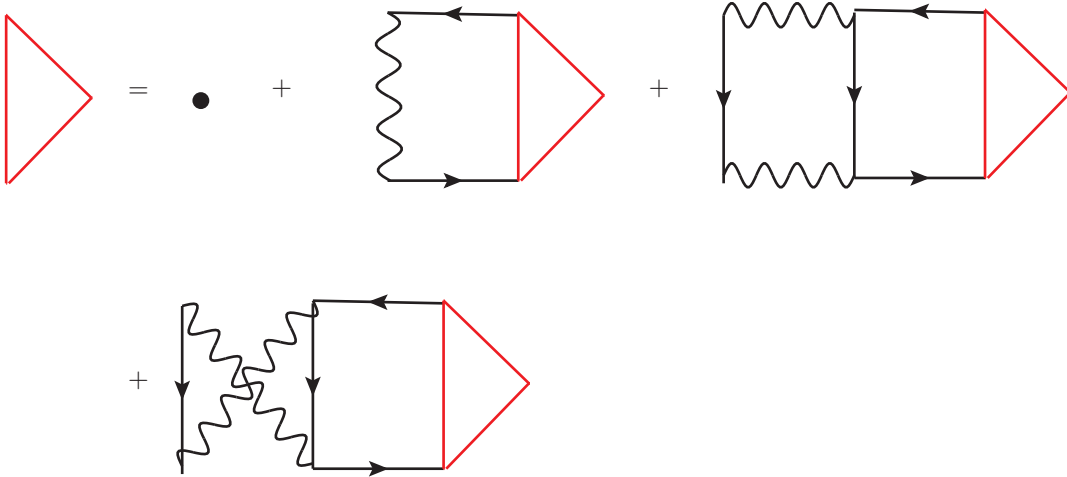
and

$$\begin{aligned} \frac{\delta \Sigma_{XC}(1, 2)}{\delta G(4, 5)} &= i\delta(1, 4)\delta(2, 5)W(1, 2) + G(1, 2)W(1, 4)G(5, 4)W(5, 2) \\ &\quad + G(1, 2)W(1, 5)G(5, 4)W(4, 2) \end{aligned} \quad (2.131)$$

Diagrammatically, equation 2.131 is:

$$\frac{\Sigma_{XC}^{GW}}{\delta G} = \text{[diagram: wavy line]} + \text{[diagram: square loop with wavy lines]} + \text{[diagram: two vertical wavy lines connected by a horizontal wavy line]}$$

then:



This approximation also results in a complex diagrammatic structure for χ .

These three conserving approximations will be used in numerical calculations to illustrate the validity of the frequency sum-rule and analyze the peak structure of χ in the following chapter.

3 Numerical illustrations

Introduction

In this chapter numerical treatments of the many-body problem will be presented shortly. A computer code based on the algorithm of time propagation of the Kadanoff-Baym equations and another code which uses the exact diagonalization method will both be used to determine numerically the quantities involved in the frequency sum-rule for small Hubbard chains to verify that the relation is satisfied and also to determine the optical spectrum of the unperturbed system.

3.1 The Green's functions code

The numerical illustrations presented in this work were obtained by using the algorithm and computer code developed by Robert van Leeuwen et. al. which solves the Kadanoff-Baym equations numerically using the time-propagation method.

The calculations are carried out using a set of basis functions:[14]

$$G(\vec{x}t, \vec{x}'t') = \sum_{ij} \phi_i(\vec{x}) G_{ij}(t, t') \phi_j^*(\vec{x}') \quad (3.1)$$

With this, all the quantities in the equations become time-dependent matrices and all products are to be interpreted as matrix products. The basis functions are represented themselves as linear combinations of Slater determinants. In the end the observables calculated from the Green's functions will not depend on whether the basis functions are obtained using Density functional theory or other methods but on the Slater basis[14].

The first stage of the calculation consists of solving to self-consistency the Dyson equation to obtain the Matsubara Green's function G^M :

$$G^M(\tau) = G_0(\tau) + \int_0^\beta d\tau' \int_0^\beta d\tau'' G_0(\tau - i\tau') \Sigma^*(\tau' - \tau'') G^M(\tau'') \quad (3.2)$$

where G_0 is the reference Green's function which is known (the physical observables calculated from the Green's function will be independent of the choice of G_0 as long as it satisfies the correct boundary conditions[14]). Also, because the Green's function is a quantity peaked around the points $\tau = 0$ and $\tau = \pm\beta$, it is calculated on a uniform-power mesh which is dense around the endpoints.

After the ground state Green's function is calculated, it can be propagated according to the Kadanoff-Baym equations, i.e. the values of the Green's function on the real part of the contour are calculated also. For example, to make the time step $G^>(T, t') \rightarrow G^>(T + \Delta, t')$, time-evolution operators of the form

$$U(\Delta) = e^{-i\bar{h}\Delta} \quad (3.3)$$

and

$$V(\Delta) = (\bar{h})^{-1}(1 - e^{-i\bar{h}\Delta}) \quad (3.4)$$

are defined where \bar{h} is the one-body part of the Hamiltonian calculated at the time $T + \frac{\Delta}{2}$. It can be proven (see reference [15]) that for a small Δ :

$$G^>(T + \Delta, t') = U(\Delta)G^>(T, t') - V(\Delta)I_1^>(T, t') \quad (3.5)$$

where I_1 is a collision integral defined as:

$$I_1^>(t, t') = \int_0^t d\bar{t} \Sigma^R(t, \bar{t}) G^>(\bar{t}, t') + \int_0^{t'} d\bar{t} \Sigma^>(t, \bar{t}) G^A(\bar{t}, t') + \frac{1}{i} \int_0^\beta d\bar{t} \Sigma^>(t, -i\bar{t}) G^>(-i\bar{t}, t') \quad (3.6)$$

Similar relations allow the calculation of the other Keldysh components of the Green's function. Then the newly calculated Green's function in $T + \Delta$ serves as the initial point of the following time step and so on.

3.2 The exact diagonalization code

The Hamiltonian of a system of noninteracting fermions on a lattice of N sites can be represented in second quantization by:

$$\hat{H}_0 = \sum_{i,j=1}^N t_{ij} \hat{c}_i^\dagger \hat{c}_j \quad (3.7)$$

where \hat{c}_i^\dagger creates a fermion in a single-particle orbital ϕ_j localized at site j and:

$$t_{ij} = \langle \phi_i | \left(-\frac{\hbar^2 \nabla^2}{2m} + \hat{v} \right) | \phi_j \rangle \quad (3.8)$$

For many practical purposes it suffices to assume that t_{ij} is non-zero only when i, j are nearest neighbors in which case it is usually denoted by $-t$ so that the Hamiltonian written in manifestly hermitian format becomes[16]:

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \quad (3.9)$$

The most general form of the interaction between the electrons in second quantization representation which can be added to \hat{H}_0 is of the form:

$$\hat{V} = \frac{1}{2} \sum_{\mu\nu\beta\alpha} V_{\mu\nu\beta\alpha} \hat{c}_\mu^\dagger \hat{c}_\nu^\dagger \hat{c}_\alpha \hat{c}_\beta \quad (3.10)$$

where $\alpha = \{\sigma, i\}$ is a collective name for the site index i and spin index σ and

$$V_{\mu\nu\beta\alpha} = \int dx dx' \phi_\mu^*(x) \phi_\nu^*(x) V(|x - x'|) \phi_\beta(x) \phi_\alpha(x') \quad (3.11)$$

The most important term among all possible $\mu\nu\beta\alpha$ matrix elements is when all the indices correspond to the same site j . In that case, the Pauli principle forces $\mu = \alpha = \uparrow$ and $\beta = \nu = \downarrow$. Denoting the corresponding matrix element with $-2U$ one gets for the screened interaction[16]:

$$V = -U \sum_j \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow} = U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (3.12)$$

If this term is added to \hat{H}_0 , the Hubbard model is obtained:

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + U \sum_j n_{j\uparrow} n_{j\downarrow} \quad (3.13)$$

To perform the exact diagonalization, a complete orthogonal basis φ_i is chosen. It can be introduced in the time independent Schrödinger equation to yield:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \quad (3.14)$$

$$\sum_j \underbrace{\langle \varphi_i | \hat{H} | \varphi_j \rangle}_{\equiv H_{ij}} \langle \varphi_j | \Psi \rangle = E \underbrace{\langle \varphi_i | \Psi \rangle}_{\equiv c_i} \quad (3.15)$$

$$\sum_j H_{ij} c_j = E c_i \quad (3.16)$$

Therefore if one can construct the Hamiltonian matrix H_{ij} , the problem is reduced to the diagonalization of a matrix. Then, assuming that at time $t_0 = 0$ the system is in the ground state $|\Psi_0\rangle$ which has been determined, if a time independent perturbation \hat{V} is switched on, the time evolution of the system can be expressed in the following way:

$$|\Psi(t)\rangle = e^{-i(\hat{H}+\hat{V})t} |\Psi_0\rangle \quad (3.17)$$

$$= \sum_j |\Phi_j\rangle \langle \Phi_j | e^{-i(\hat{H}+\hat{V})t} | \Psi_0 \rangle \quad (3.18)$$

$$= \sum_j |\Phi_j\rangle e^{-iE_j t} \langle \Phi_j | \Psi_0 \rangle \quad (3.19)$$

where Φ_j are the eigenstates of the Hamiltonian $\hat{H} + \hat{V}$ with corresponding eigenenergies E_j which can be determined using the same diagonalization procedure as before.

A delta-kick perturbation of the form:

$$\hat{V} = \lim_{\Delta \rightarrow 0} \frac{\lambda}{\Delta} \hat{A} \quad (3.20)$$

where \hat{A} is a time independent operator, leads after a time Δ to:

$$|\Psi(\Delta)\rangle = e^{-i(\hat{H}+\hat{V})\Delta} |\Psi_0\rangle \quad (3.21)$$

$$= e^{-i\hat{H}\Delta + \lambda\hat{A}} |\Psi_0\rangle \quad (3.22)$$

which, in the limit $\Delta \rightarrow 0$:

$$\lim_{\Delta \rightarrow 0^+} \Psi(\Delta) = e^{-i\lambda\hat{A}} |\Psi_0\rangle = |\tilde{\Psi}_0\rangle \quad (3.23)$$

Therefore, the time-evolution of the system which was perturbed at $t=0$ with a delta kick potential can be determined by solving the Schrödinger equation for the unperturbed Hamiltonian:

$$i\partial_t |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \quad (3.24)$$

with the initial condition:

$$|\Psi(0)\rangle = |\tilde{\Psi}_0\rangle \quad (3.25)$$

i.e.

$$|\Psi(t)\rangle = \sum_j e^{-i\epsilon_j t} \langle \Psi_j | \tilde{\Psi}_0 \rangle |\Psi_j\rangle \quad (3.26)$$

where

$$\hat{H} |\Psi_j\rangle = \epsilon_j |\Psi_j\rangle \quad (3.27)$$

3.3 Verifying numerically the frequency sum-rule

The frequency sum-rule was derived to be:

$$-\partial_t \chi_{ij}^R(0^+) = h_{ij} \gamma_{ji} + h_{ji} \gamma_{ij} - \delta_{ij} \sum_k (h_{ik} \gamma_{ki} + h_{ki} \gamma_{ik}) \quad (3.28)$$

where

$$\gamma_{ij} = \langle \hat{a}_j^\dagger \hat{a}_i \rangle \quad (3.29)$$

h_{ij} are the matrix elements of the unperturbed one-particle Hamiltonian and χ_{ij}^R is the retarded density response function.

The Hubbard model Hamiltonian was used. For a six-site system:

$$h_{ij} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (3.30)$$

The frequency sum-rule was verified numerically for systems of Hubbard chains consisting of 2, 4 and 6 sites. The Hubbard interaction parameter U (see equation 3.13) was taken to be 1 a.u. The system was perturbed with a delta function potential:

$$v_{ij}(t) = \lambda \sum_{ij}^N \delta_{1i} \delta_{ij} \delta(t) \quad (3.31)$$

of intensity $\lambda = 0.05 a.u.$, which is a weak enough perturbation to enable the study of the linear response of the system. The perturbation was applied at site 1.

In this case

$$\chi^R(t) = \frac{\delta n(t)}{\lambda} \quad (3.32)$$

The change in density at site 1 as a consequence of the delta-kick was recorded to yield the first component of the $\chi^R(t)$ matrix, i.e. $\chi_{11}^R(t)$.

First the density as a function of time and the gamma matrices in the sum-rule were calculated with the Green's functions code using the Hartree-Fock (HF), second Born (2B) and GW approximations for the self-energy.

$$\gamma_{ij} = -i G_{ij}(0, 0^+) \quad (3.33)$$

To calculate the derivative in the l.h.s. of equation 3.28 a very small time step of $10^{-6} a.u.$ was used to propagate the KB equations and obtain the change in density after which the tangent was calculated with the usual formula:

$$\partial_t \chi^R(0^+) = \frac{1}{\lambda} \frac{n(0 + \Delta t) - n(0)}{\Delta t} \quad (3.34)$$

Then these quantities were re-calculated with the exact diagonalization code for the same input parameters as for the Green's functions code, i.e. $U = 1 a.u.$, $\Delta t = 10^{-6} a.u.$, $\lambda = 0.05 a.u.$ and with the same h_{ij} matrix. The results are shown in the following table:

2 sites	$x = -\partial_t \chi_{11}^R(0^+)(a.u.)$	y=r.h.s (a.u.)	relative error $\Delta = \frac{x-y}{x}$
HF	0.99958	1.00000	0.04%
2B	0.97301	0.97342	0.04%
GW	0.97306	0.97347	0.04%
EXACT	0.96973	0.97014	0.04%
4 sites	$x = -\partial_t \chi_{11}^R(0^+)(a.u.)$	y=r.h.s (a.u.)	relative error $\Delta = \frac{x-y}{x}$
HF	0.89405	0.89442	0.04%
2B	0.87588	0.87624	0.04%
GW	0.87670	0.87706	0.04%
EXACT	0.87279	0.87315	0.04%
6 sites	$x = -\partial_t \chi_{11}^R(0^+)(a.u.)$	y=r.h.s (a.u.)	relative error $\Delta = \frac{x-y}{x}$
HF	0.87075	0.87111	0.04%
2B	0.85482	0.85517	0.04%
GW	0.85557	0.85593	0.04%
EXACT	0.85180	0.85215	0.04%

The frequency sum-rule is satisfied to the same extent by all the approximations as by the exact diagonalization calculation. 2B and GW approximations yield sumrule values closer to the exact ones than the HF approximation. The relative error is the same for all approximations based calculations as for the exact one and its value is not a consequence of the number of diagram classes taken into account in the expression for the self-energy nor of the numerical errors induced by the codes. It resulted from the way the limit of the derivative in the l.h.s of the sum-rule was calculated. It can be reduced by considering a smaller time step and also by using a more powerful formula for the numerical calculation of a derivative than equation 3.34. However, the purpose was not to achieve the highest numerical accuracy since of course it can be proven analytically that the sum-rule is valid (as was shown in the previous chapter). These numerics serve only as an illustration. It is noteworthy though that the Green's function code was as adequate as the exact diagonalization code in demonstrating the validity of the frequency sum-rule under the same accuracy demands and the same input parameters.

3.4 Optical spectra numerical calculations

An interesting property to illustrate numerically that the response function possesses is that its Fourier transform has peaks corresponding to the optical spectrum of the unperturbed system (equations 2.43, 2.44). This property cannot be proven for χ calculated using approximations for the self-energy. However, in this case also χ was shown to have a peak structure (equation 2.99) and it is worthwhile to compare it to the optical spectrum calculated with the exact diagonalization procedure.

The KB equations were propagated for a longer period of time (100 a.u. with a time step of 0.1 a.u.) and the change in density at site 1 was recorded after applying a delta-kick perturbation of 0.05 a.u. at site 1 for Hubbard chains (U=1) of 2, 4 and 6 sites. And for the same parameters the probability density at site 1 was also calculated with the exact diagonalization code. The results are plotted in figures 1, 2 and 3.

In the previous case, when checking the frequency sum-rule all the approximations performed equally well. Now, the number of diagram classes taken into account by a conserving approximation comes into play. It can be noticed that both the HF and 2B approximations deviate from the exact diagonalization result and moreover, HF deviates more severely than 2B, since it takes into account less diagrams than 2B does.

Also, at the beginning of the propagation the approximations are closer to the exact value than at later times. As time passes the deviation becomes more and more obvious. According to equation 2.34:

$$i\chi_{ij}^R(t-t') = \sum_s e^{i(E_0 - E_{N,s})(t-t')} (\langle \Psi_0 | \hat{n}_i | \Psi_0 \rangle \langle \Psi_0 | \hat{n}_j | \Psi_0 \rangle - \langle \Psi_0 | \hat{n}_j | \Psi_0 \rangle \langle \Psi_0 | \hat{n}_i | \Psi_0 \rangle) \quad (3.35)$$

Then, if the eigenenergies E_0 , $E_{N,s}$ calculated within an approximation differ even slightly from the exact values, i.e. by δE , the phase factor $e^{i\delta E t}$ will cause the approximate response function to grow out of phase with respect to the exact response function (after $\delta t = \frac{\pi}{\delta E}$, the two functions will be in antiphase).

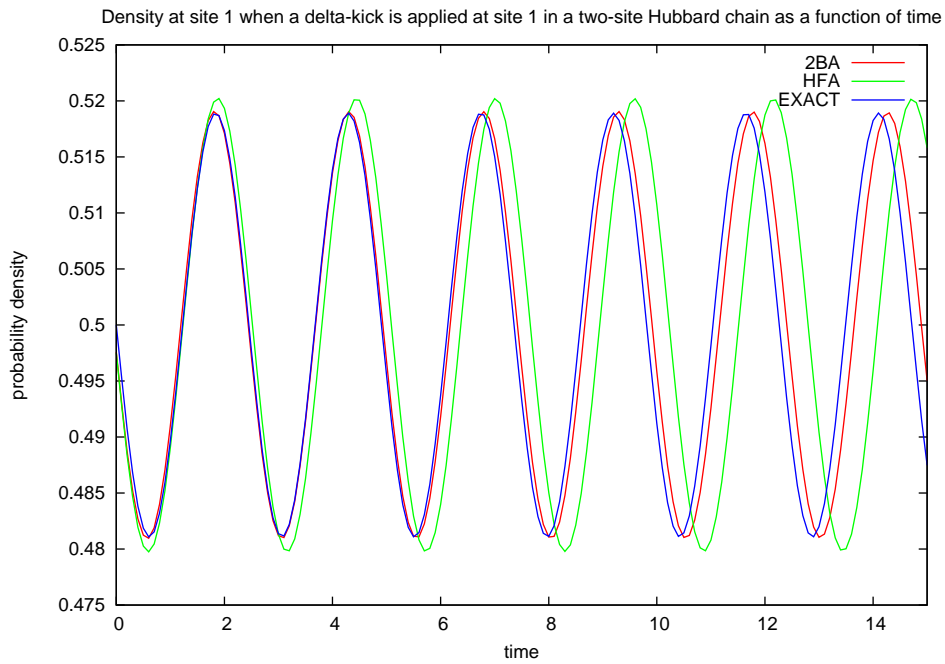


Figure 1: Density at site 1 as a function of time in a 2 site Hubbard chain ($U=1$) when a delta-kick perturbation of 0.05 a.u. is applied at site 1

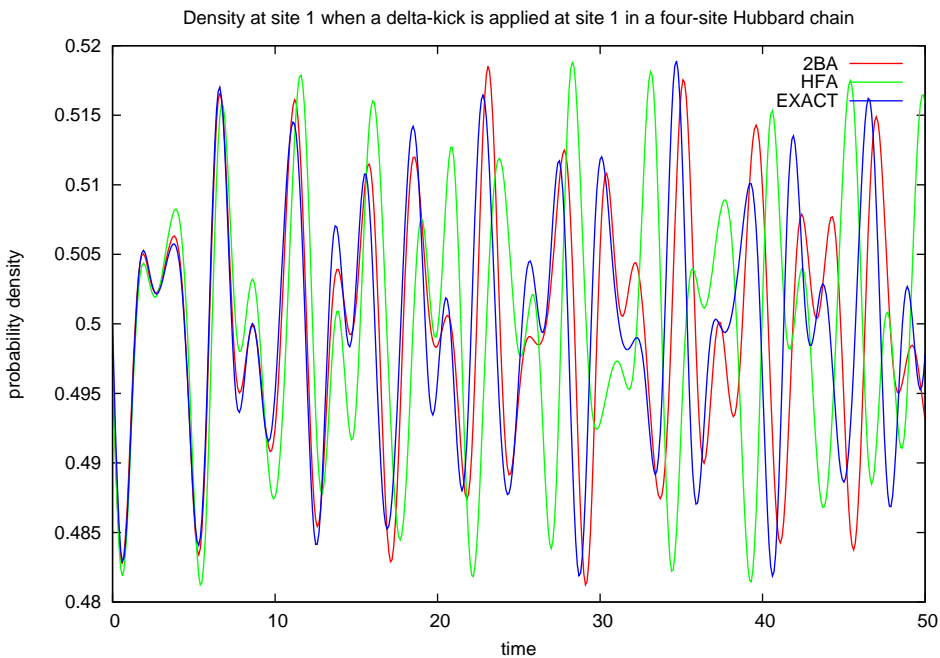


Figure 2: Density at site 1 as a function of time in a 4 site Hubbard chain ($U=1$) when a delta-kick perturbation of 0.05 a.u. is applied at site 1

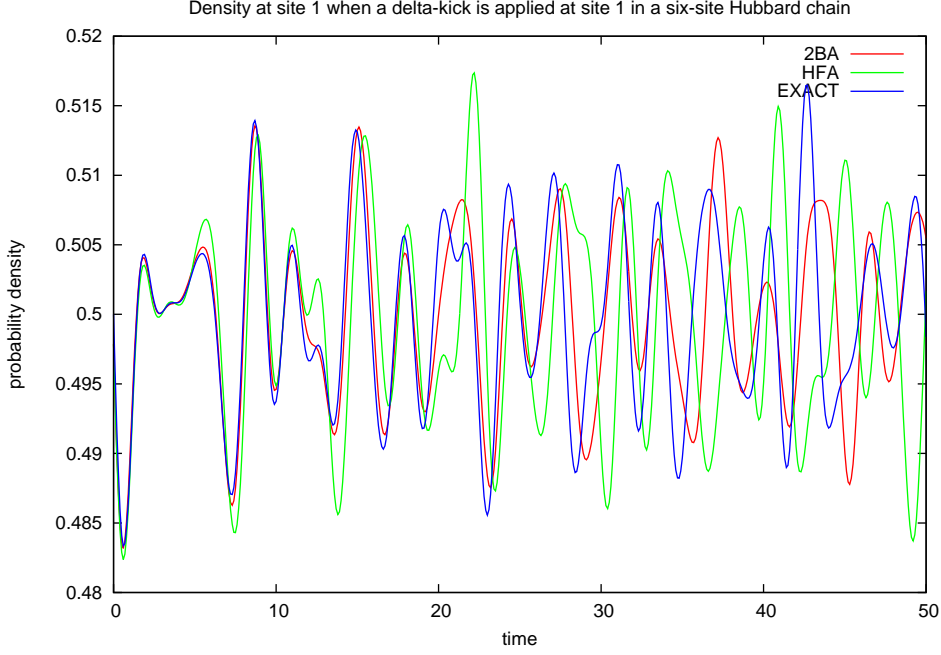


Figure 3: Density at site 1 as a function of time in a 6 site Hubbard chain ($U=1$) when a delta-kick perturbation of 0.05 a.u is applied at site 1

After the propagation, the Fourier transform of the function χ was plotted against the values of the energy differences corresponding to allowed transitions in the unperturbed system spectrum calculated with the exact diagonalization code. The Fourier transform of χ calculated with the exact diagonalization code is plotted also to see how much of the difference in the values of the peaks from the exact spectrum comes from too short propagation in time for the Fourier transform. The finite-time Fourier transform is:

$$f_T(\omega) = \int_0^T dt e^{i\omega t} f(t) \quad (3.36)$$

where T should be as large as possible ($T \rightarrow \infty$)

As it can be seen from figures 4 and 5, the peaks calculated using the 2B approximation are closer to the exact value than those calculated with HF which shows the superiority of MBPT schemes over the mean-field method. For some peaks, however, the results are inconclusive, the cause for this being a too-short time propagation before taking the Fourier transform. The relative errors in the estimation of the peak positions are given in the following table.

2 sites	HF	2B
peak	4%	1%
4 sites	HF	2B
first peak	6%	1%
second peak	3%	1%
third peak	1%	inconclusive
6 sites	HF	2B
first peak	8%	2.6%
second peak	3.4%	1.4%
third peak	1.4%	inconclusive
fourth peak	1.2%	inconclusive

Still, it is obvious from these numerical results that the peak structure of the response function in Fourier space calculated with the Green's function method within the conserving approximations does tend towards the energy peaks of the optical spectrum of the system.

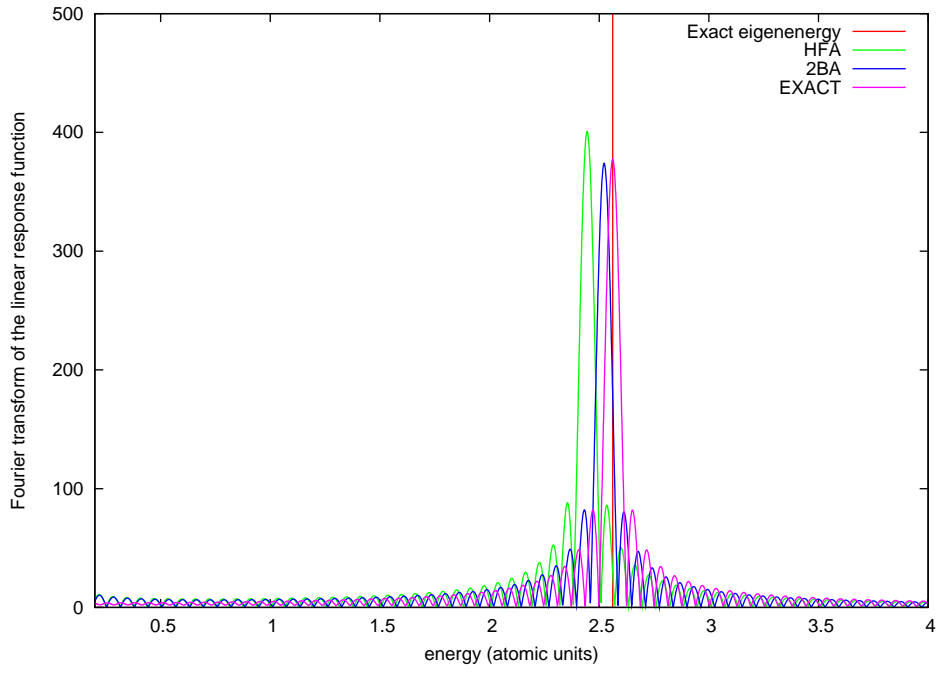


Figure 4: Fourier transform of the density response function for a two-site Hubbard system ($U=1$)

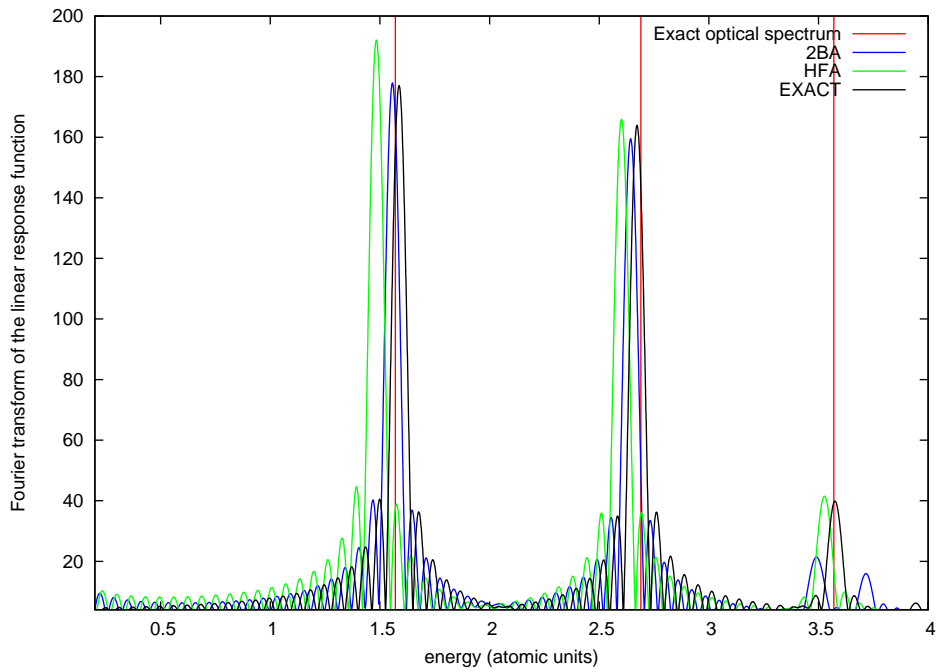


Figure 5: Fourier transform of the density response function for a four-site Hubbard system ($U=1$)

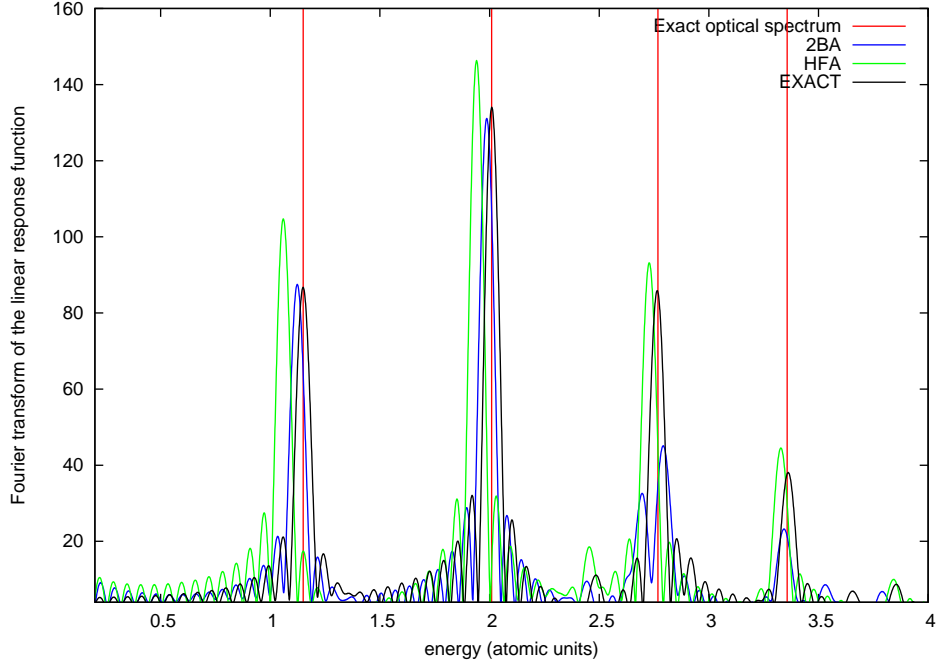


Figure 6: Fourier transform of the density response function for a six-site Hubbard system ($U=1$)

4 Conclusions

1. MBPT allows a systematic inclusion of electronic interactions
2. Approximations can be chosen in a conserving way, ensuring the satisfaction of macroscopic conservation laws and of the frequency sumrule.
3. Propagation of the Kadanoff-Baym equations within relatively simple self-energy approximations leads to very sophisticated response functions involving a Bethe-Salpeter equation with a kernel $\frac{\delta \Sigma}{\delta G}$. This way of using MBPT goes much beyond existing approaches based on equilibrium theory.
4. The many-body approaches show a clear improvement over the mean-field Hartree-Fock approach.
5. Efficient schemes need to be developed to perform long-time propagations with the Kadanoff-Baym equations to extract detailed optical spectra.

A Appendix

A.1 Anticommutation relations between fermionic field operators

$$\{\hat{\psi}^\dagger(\vec{x}), \hat{\psi}(\vec{x}')\} = \delta(\vec{x} - \vec{x}') \quad (\text{A.1})$$

Proof.

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

Adding the two results gives:

$$\left(\hat{\psi}(\vec{x}')\hat{\psi}^\dagger(\vec{x}) + \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x}')\right)\Psi_n = \delta(\vec{x} - \vec{x}')\Psi_n$$

□

$$\{\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}')\} = 0$$

Proof.

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

where in the last line the antisymmetry of the wave-function was used.

Therefore,

$$\left(\hat{\psi}(\vec{x})\hat{\psi}(\vec{x}') + \hat{\psi}(\vec{x}')\hat{\psi}(\vec{x})\right)\Psi_n = 0$$

□

Taking the adjoint of this last equation yields:

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

A.2 One-body and two-body operators in terms of field operators

$$\hat{O} = \sum_i \hat{o}(\vec{x}_i) = \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{o}(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{A.2})$$

Proof.

$$\begin{aligned} \int d\vec{x} \hat{\psi}^\dagger(\vec{x}) \hat{o}(\vec{x}) \hat{\psi}(\vec{x}) \Psi_n &= \int d\vec{x} \hat{o}(\vec{x}') \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x}') \Big|_{\vec{x}'=\vec{x}} \Psi_n \\ &= \int d\vec{x} \hat{o}(\vec{x}') \sum_{j=1}^n \delta(\vec{x} - \vec{x}_j) \Psi_n(\vec{x}_1, \dots, \vec{x}_{j-1}, \vec{x}', \vec{x}_{j+1}, \dots, \vec{x}_n) \Big|_{\vec{x}'=\vec{x}} \\ &= \sum_{j=1}^n \hat{o}(\vec{x}_j) \Psi_n = \hat{O} \Psi_n \end{aligned}$$

□

For two-body operators:

$$\begin{aligned} \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \hat{\psi}(\vec{y}) \hat{\psi}(\vec{x}) \Psi_n &= \sqrt{n} \sqrt{n-1} \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{y}) \\ &\Psi_n(\vec{x}_1, \dots, \vec{x}_{n-2}, \vec{y}, \vec{x}) \\ &= \sqrt{n} \sqrt{n-1} \hat{\psi}^\dagger(\vec{x}) \frac{(-1)^{n-2}}{\sqrt{n-1}} \sum_{j=1}^{n-1} (-1)^{j+1} \delta(\vec{y} - \vec{x}_j) \\ &\Psi_n(\vec{x}_1, \dots, \hat{x}_j, \vec{x}_{n-1}, \vec{y}, \vec{x}) \\ &= \sqrt{n} (-1)^n \hat{\psi}^\dagger(\vec{x}) \sum_{j=1}^{n-1} (-1)^{n-1-j} (-1)^{j+1} \delta(\vec{y} - \vec{x}_j) \\ &\Psi_n(\vec{x}_1, \dots, \vec{x}_{j-1}, \vec{y}, \vec{x}_{j+1}, \dots, \vec{x}_{n-1}, \vec{x}) \\ &= \sqrt{n} \hat{\psi}^\dagger(\vec{x}) \sum_{j=1}^{n-1} \delta(\vec{y} - \vec{x}_j) \\ &\Psi_n(\vec{x}_1, \dots, \vec{x}_{j-1}, \vec{y}, \vec{x}_{j+1}, \dots, \vec{x}_{n-1}, \vec{x}) \\ &= \sqrt{n} \sum_{j=1}^{n-1} \delta(\vec{y} - \vec{x}_j) \frac{(-1)^{n-1}}{\sqrt{n}} \sum_{k=1}^n (-1)^{k+1} \delta(\vec{x} - \vec{x}_k) \\ &\Psi_n(\vec{x}_1, \dots, \hat{x}_k, \dots, \vec{x}_n, \vec{x}) \\ &= (-1)^{n-1} \sum_{j=1}^{n-1} \sum_{k=1}^n \delta(\vec{y} - \vec{x}_j) \delta(\vec{x} - \vec{x}_k) (-1)^{k+1} (-1)^{n-k} \\ &\Psi_n(\vec{x}_1, \dots, \hat{x}_n) \\ &= \sum_{j \neq k}^n \delta(\vec{y} - \vec{x}_j) \delta(\vec{x} - \vec{x}_k) \Psi_n \end{aligned}$$

A.3 Solving the integral equation for the time-evolution operator using the reciprocal kernel method

$$\hat{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{V}_I(t') \hat{U}(t', t_0) \quad (\text{A.3})$$

This is a Volterra integral equation of the second kind:

$$\phi(x) = f(x) + \lambda \int_0^x K(x, u) \phi(u) du \quad (\text{A.4})$$

The reciprocal kernel method[2]

Seek the solution by means of a power series in λ :

$$\phi(x) = \sum_{n=0}^{\infty} \lambda^n \phi_n(x) \quad (\text{A.5})$$

Substitute this series into the integral equation:

$$\phi_0(x) + \lambda \phi_1(x) + \lambda^2 \phi_2(x) + \lambda^3 \phi_3(x) + \dots = \quad (\text{A.6})$$

$$f(x) + \lambda \int_0^x K(x, u) \phi_0(u) du + \lambda^2 \int_0^x K(x, u) \phi_1(u) du + \lambda^3 \int_0^x K(x, u) \phi_2(u) du + \dots \quad (\text{A.7})$$

Compare the coefficients of equal powers of λ :

$$\phi_0(x) = f(x) \quad (\text{A.8})$$

$$\phi_1(x) = \int_0^x K(x, u) \phi_0(u) du = \int_0^x K(x, u) f(u) du \quad (\text{A.9})$$

$$\phi_2(x) = \int_0^x K(x, u) \phi_1(u) du = \int_0^x K(x, u) \left(\int_0^u K(u, v) f(v) dv \right) du \quad (\text{A.10})$$

$$= \int_0^x \underbrace{\left(\int_v^x K(x, u) K(u, v) du \right)}_{\equiv K_2(x, v)} f(v) \quad (\text{A.11})$$

$$= \int_0^x K_2(x, v) f(v) dv \quad (\text{A.12})$$

Generally,

$$\phi_n(x) = \int_0^x K_n(x, u) f(u) du \quad (\text{A.13})$$

$K_n(x, u)$ are called iterated kernels and are determined by the recursion formulas:

$$K_1(x, u) = K(x, u) \quad (\text{A.14})$$

$$K_{n+1}(x, u) = \int_u^x K(x, y) K_n(y, u) dy \quad (\text{A.15})$$

From:

$$\phi(x) = \sum_{n=0}^{\infty} \lambda^n \phi_n(x)$$

we have:

$$\phi(x) = f(x) + \sum_{n=1}^{\infty} \lambda^n \int_0^x K_n(x, u) f(u) du \quad (\text{A.16})$$

$$= f(x) + \lambda \int_0^x \underbrace{\sum_{n=0}^{\infty} \lambda^n K_{n+1}(x, u) f(u) du}_{\equiv R(x, u; \lambda)} \quad (\text{A.17})$$

$$R(x, u; \lambda) = \sum_{n=0}^{\infty} \lambda^n K_{n+1}(x, u) \quad (\text{A.18})$$

is called the Liouville-Neumann series representing the reciprocal kernel, or resolvent kernel of the integral equation.

The solution of the integral equation becomes:

$$\phi(x) = f(x) + \lambda \int_0^x R(x, u; \lambda) f(u) du \quad (\text{A.19})$$

In this case:

$$\hat{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{V}_I(t') \hat{U}(t', t_0) \quad (\text{A.20})$$

$$f(x) = 1 \quad (\text{A.21})$$

$$K_1(t_1) = \hat{V}_I(t_1) \quad (\text{A.22})$$

$$K_2(t_1) = \int_{t_1}^t \hat{V}_I(t_2) \hat{V}_I(t_1) dt_2 \quad (\text{A.23})$$

$$K_3(t_1) = \int_{t_1}^t \hat{V}_I(t_3) \int_{t_1}^{t_3} \hat{V}_I(t_2) \hat{V}_I(t_1) dt_2 dt_3 \quad (\text{A.24})$$

In general:

$$K_{n+1}(t_1) = \int_{t_1}^t \hat{V}_I(t_{n+1}) \int_{t_1}^{t_{n+1}} \hat{V}_I(t_n) \int_{t_1}^{t_n} \hat{V}_I(t_{n-1}) \dots \int_{t_1}^{t_3} \hat{V}_I(t_2) \hat{V}_I(t_1) dt_2 dt_3 \dots dt_{n+1} \quad (\text{A.25})$$

Using the identity:

$$\int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \hat{O}(t_1) \dots \hat{O}(t_n) = \frac{1}{n!} \int_{t_0}^t dt_1 \dots dt_n T[\hat{O}(t_1) \dots \hat{O}(t_n)] \quad (\text{A.26})$$

$$\begin{aligned} R(t_1) &= \hat{V}_I(t_1) + \left(-\frac{i}{\hbar}\right) \int_{t_1}^t \hat{V}_I(t_2) \hat{V}_I(t_1) dt_2 \\ &+ \left(-\frac{i}{\hbar}\right)^2 \cdot \frac{1}{2} \int_{t_1}^t dt_2 dt_3 T[\hat{V}_I(t_3) \hat{V}_I(t_2) \hat{V}_I(t_1)] + \dots \\ &+ \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{t_1}^t dt_2 \dots dt_n T[\hat{V}_I(t_n) \dots \hat{V}_I(t_1)] \end{aligned}$$

Then:

$$\begin{aligned} \hat{U}(t, t_0) &= 1 - \frac{i}{\hbar} \int_{t_0}^t R(t_1) dt_1 = 1 + \left(-\frac{i}{\hbar}\right) \int_{t_0}^t \hat{V}_I(t_1) dt_1 \\ &+ \left(-\frac{i}{\hbar}\right)^2 \cdot \frac{1}{2} \int_{t_0}^t dt_1 dt_2 T[\hat{V}_I(t_1) \hat{V}_I(t_2)] + \dots \\ &+ \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \dots dt_n T[\hat{V}_I(t_n) \dots \hat{V}_I(t_1)] + \dots \\ &= T\left[\exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' \hat{V}_I(t')\right)\right] \quad (\text{A.27}) \end{aligned}$$

A.4 Proof of the Gell-Mann and Low theorem

This proof represents a summary of the proof from the paper by Luca Guido Molinari (reference [5]).

In the appendix of their paper, "Bound States in Quantum Field Theory", Murray Gell-Mann and Francis Low proved a fundamental theorem that connects the ground states $|\Psi_0\rangle$ and $|\Psi\rangle$ of Hamiltonians \hat{H}_0 and $\hat{H} = \hat{H}_0 + g\hat{V}$. The theorem introduces the concept of adiabatic switching on of the interaction, the Hamiltonian used being of the form:

$$H_\epsilon(t) = H_0 + e^{-\epsilon|t|}gV \quad (\text{A.28})$$

The statement of the theorem is the following:

Theorem (Gell-Mann and Low). *Let $|\Psi_0\rangle$ be an eigenstate of H_0 with eigenvalue E_0 and consider the vectors:*

$$|\Psi_\epsilon^{(\pm)}\rangle = \frac{\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle}{\langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle}$$

If the limit vectors $|\Psi^{(\pm)}\rangle$ for $\epsilon \rightarrow 0^+$ exists, then they are eigenstates of \hat{H} with the same eigenvalue E .

To prove it, the following lemma was used:

Lemma. *If $\hat{U}_\epsilon(t, s)$ is the time propagator for $\hat{H}_\epsilon(t)$, then for all positive ϵ , the following relations hold:*

$$i\hbar\epsilon g \frac{\partial}{\partial g} \hat{U}_\epsilon(t, s) = \begin{cases} \hat{H}_\epsilon(t)\hat{U}_\epsilon(t, s) - \hat{U}_\epsilon(t, s)\hat{H}_\epsilon(s) & \text{if } 0 \geq t \geq s \\ -\hat{H}_\epsilon(t)\hat{U}_\epsilon(t, s) + \hat{U}_\epsilon(t, s)\hat{H}_\epsilon(s) & \text{if } t \geq s \geq 0 \end{cases}$$

Proof. From the Schrödinger equation:

$$i\hbar\partial_t \hat{U}_\epsilon(t, s) = \hat{H}_\epsilon(t)\hat{U}_\epsilon(t, s) \quad (\text{A.29})$$

with:

$$\hat{U}_\epsilon(s, s) = 1 \quad (\text{A.30})$$

an integral equation can be obtained:

$$\hat{U}_\epsilon(t, s) = 1 + \frac{1}{i\hbar} \int_s^t dt' \left(\hat{H}_0 + e^{\epsilon(\theta - |t'|)}\hat{V} \right) \hat{U}_\epsilon(t', s) \quad (\text{A.31})$$

where:

$$g = e^{\epsilon\theta} \quad (\text{A.32})$$

Consider the g -independent operators $\hat{H}^{(\pm)}(t) = \hat{H}_0 + e^{\pm\epsilon t}\hat{V}$ with corresponding propagators $\hat{U}^{(\pm)}(t, s)$. For $0 \geq t \geq s$ a time translation in equation A.31 yields:

$$\hat{U}_\epsilon(t, s) = 1 + \frac{1}{i\hbar} \int_{s+\theta}^{t+\theta} dt' \hat{H}^{(+)}(t')\hat{U}_\epsilon(t' - \theta, s) \quad (\text{A.33})$$

On the other hand,

$$\hat{U}^{(+)}(t + \theta, s + \theta) = 1 + \frac{1}{i\hbar} \int_{s+\theta}^{t+\theta} dt' \hat{H}^{(+)}(t')\hat{U}^{(+)}(t', s + \theta) \quad (\text{A.34})$$

The unicity of the solution of the Schrödinger equation implies:

$$\hat{U}_\epsilon(t, s) = \hat{U}^{(+)}(t + \theta, s + \theta) \quad (\text{A.35})$$

Since θ enters in the operator $\hat{U}^{(+)}(t + \theta, s + \theta)$ only in its temporal variables, then:

$$\partial_\theta \hat{U}_\epsilon(t, s) = \partial_t \hat{U}_\epsilon(t, s) + \partial_s \hat{U}_\epsilon(t, s) \quad (\text{A.36})$$

Further,

$$\begin{aligned}
i\hbar\partial_t\hat{U}_\epsilon(t,s) &= \hat{H}_\epsilon(t)\hat{U}_\epsilon(t,s) \\
-i\hbar\partial_t\hat{U}_\epsilon^\dagger(t,s) &= \hat{U}_\epsilon^\dagger(t,s)\hat{H}_\epsilon(t) \\
\hat{U}_\epsilon^\dagger(t,s) &= \hat{U}_\epsilon^{-1}(t,s) = \hat{U}_\epsilon(s,t) \\
-i\hbar\partial_s\hat{U}_\epsilon(t,s) &= \hat{U}_\epsilon(t,s)\hat{H}_\epsilon(s)
\end{aligned}$$

which makes:

$$\partial_\theta\hat{U}_\epsilon(t,s) = \frac{1}{i\hbar} \left(\hat{H}_\epsilon(t)\hat{U}_\epsilon(t,s) - \hat{U}_\epsilon(t,s)\hat{H}_\epsilon(s) \right) \quad (\text{A.37})$$

Then,

$$\begin{aligned}
i\hbar\epsilon g \frac{\partial}{\partial g} \hat{U}_\epsilon(t,s) &= i\hbar\epsilon e^{\epsilon\theta} \frac{\partial\theta}{\partial g} \partial_\theta \hat{U}_\epsilon(t,s) = \\
i\hbar\partial_\theta \hat{U}_\epsilon(t,s) &= \hat{H}_\epsilon(t)\hat{U}_\epsilon(t,s) - \hat{U}_\epsilon(t,s)\hat{H}_\epsilon(s)
\end{aligned}$$

If $t \geq s \geq 0$ the same procedure gives $\hat{U}_\epsilon(t,s) = \hat{U}_\epsilon^{(-)}(t-\theta, s-\theta)$ and therefore:

$$\partial_\theta \hat{U}_\epsilon(t,s) = -\partial_t \hat{U}_\epsilon(t,s) - \partial_s \hat{U}_\epsilon(t,s) \quad (\text{A.38})$$

which concludes the proof of the lemma. \square

In the interaction picture:

$$i\hbar\epsilon g \frac{\partial}{\partial g} \hat{U}_{\epsilon I}(t,s) = \begin{cases} \hat{H}_{\epsilon I}(t)\hat{U}_{\epsilon I}(t,s) - \hat{U}_{\epsilon I}(t,s)\hat{H}_{\epsilon I}(s) & \text{if } 0 \geq t \geq s \\ -\hat{H}_{\epsilon I}(t)\hat{U}_{\epsilon I}(t,s) + \hat{U}_{\epsilon I}(t,s)\hat{H}_{\epsilon I}(s) & \text{if } t \geq s \geq 0 \end{cases} \quad (\text{A.39})$$

where:

$$\hat{H}_{\epsilon I}(t) = e^{i\hat{H}_0 t/\hbar} \hat{H}_\epsilon(t) e^{-i\hat{H}_0 t/\hbar} \quad (\text{A.40})$$

By applying these equations to an eigenstate $|\Psi_0\rangle$ of \hat{H}_0 and taking $t=0, s=\pm\infty$ one obtains:

$$\left(\hat{H} - E_0 \pm i\hbar\epsilon g \frac{\partial}{\partial g} \right) \hat{U}_{\epsilon I}(0, \pm\infty) |\Psi_0\rangle = 0 \quad (\text{A.41})$$

The existence of an adiabatic limit requires $\hat{U}_{\epsilon I}(0, \pm\infty) |\Psi_0\rangle$ to have a phase proportional to $\frac{1}{\epsilon}$. This singular phase will precisely be removed by the denominator in the definition of the vectors $|\Psi_\epsilon^{(\pm)}\rangle$ before the limit is taken.

Multiplying equation A.41 with $\langle\Psi_0|$ on the l.h.s. yields:

$$\begin{aligned}
& (\langle\Psi_0|\hat{H}\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle - \langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle E_0 \\
& \pm i\hbar\epsilon g \frac{\partial}{\partial g} \langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle) \cdot \frac{1}{\langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle} = 0
\end{aligned}$$

and further:

$$\langle\Psi_0|\hat{H}|\Psi_\epsilon^{(\pm)}\rangle - E_0 = \mp i\hbar\epsilon g \frac{\partial}{\partial g} \ln \langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle \quad (\text{A.42})$$

Denoting $E_\epsilon^{(\pm)} = \langle\Psi_0|\hat{H}|\Psi_\epsilon^{(\pm)}\rangle$ gives:

$$E_0 = E_\epsilon^{(\pm)} \pm i\hbar\epsilon g \frac{\partial}{\partial g} \ln \langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle \quad (\text{A.43})$$

Introduce this result into equation A.41:

$$\begin{aligned}
& [(\hat{H} - E_\epsilon^{(\pm)} \pm i\hbar\epsilon g \frac{1}{\langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle} \frac{\partial}{\partial g} \langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle) \\
& \cdot \hat{U}_{\epsilon I}(0, \pm\infty) |\Psi_0\rangle \pm i\hbar\epsilon g \frac{\partial}{\partial g} \hat{U}_{\epsilon I}(0, \pm\infty) |\Psi_0\rangle] \cdot \frac{1}{\langle\Psi_0|\hat{U}_{\epsilon I}(0, \pm\infty)|\Psi_0\rangle} = 0
\end{aligned}$$

to obtain:

$$\left(\hat{H} - E_\epsilon^{(\pm)} \pm i\hbar\epsilon g \frac{\partial}{\partial g} \right) |\Psi_\epsilon^{(\pm)}\rangle = 0 \quad (\text{A.44})$$

Then for $\epsilon \rightarrow 0^+$ the limit vectors $|\Psi^{(\pm)}\rangle$ are eigenvectors of $\hat{H} = \hat{H}_0 + g\hat{V}$ with eigenvalues E.

A.5 Proof of a very important relation in Quantum Field Theory

$$\begin{aligned} \frac{\langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} &= \frac{1}{\langle \phi_0 | \hat{U}_\epsilon(\infty, -\infty) | \phi_0 \rangle} \\ &\times \langle \phi_0 | \sum_{\nu=0}^{\infty} \left(-\frac{i}{\hbar} \right)^\nu \frac{1}{\nu!} \int_{-\infty}^{+\infty} dt_1 \dots \int_{-\infty}^{+\infty} dt_\nu e^{-\epsilon(|t_1|+\dots+|t_\nu|)} \\ &\times T[\hat{V}_I(t_1) \dots \hat{V}_I(t_\nu) \hat{O}_I(t)] | \phi_0 \rangle \end{aligned} \quad (\text{A.45})$$

Proof. According to Gell-Mann and Low's theorem, the ground state of the interaction system is:

$$\frac{|\Psi_0\rangle}{\langle \phi_0 | \Psi_0 \rangle} = \frac{\hat{U}_\epsilon(0, \pm\infty) | \phi_0 \rangle}{\langle \phi_0 | \hat{U}_\epsilon(0, \pm\infty) | \phi_0 \rangle} \quad (\text{A.46})$$

$$\frac{\langle \Psi_0 | \Psi_0 \rangle}{\langle \phi_0 | \Psi_0 \rangle^2} = \frac{\langle \phi_0 | \hat{U}_\epsilon(0, \pm\infty)^\dagger \hat{U}_\epsilon(0, \pm\infty) | \phi_0 \rangle}{|\langle \phi_0 | \Psi_0 \rangle|^2} \quad (\text{A.47})$$

$$= \frac{\langle \phi_0 | \hat{U}_\epsilon(\infty, -\infty) | \phi_0 \rangle}{|\langle \phi_0 | \Psi_0 \rangle|^2} \quad (\text{A.48})$$

Similarly,

$$\frac{\langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle}{\langle \phi_0 | \Psi_0 \rangle^2} = \langle \phi_0 | \hat{U}_\epsilon(\infty, 0) \hat{U}_\epsilon(0, t) \hat{O}_I(t) \hat{U}_\epsilon(t, 0) \hat{U}_\epsilon(0, -\infty) | \phi_0 \rangle \cdot \frac{1}{\langle \phi_0 | \Psi_0 \rangle^2} \quad (\text{A.49})$$

$$= \frac{\langle \phi_0 | \hat{U}_\epsilon(\infty, t) \hat{O}_I(t) \hat{U}_\epsilon(t, -\infty) | \phi_0 \rangle}{\langle \phi_0 | \Psi_0 \rangle^2} \quad (\text{A.50})$$

Then,

$$\frac{\langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{\langle \phi_0 | \hat{U}_\epsilon(\infty, t) \hat{O}_I(t) \hat{U}_\epsilon(t, -\infty) | \phi_0 \rangle}{\langle \phi_0 | \hat{U}_\epsilon(\infty, -\infty) | \phi_0 \rangle} \quad (\text{A.51})$$

Using the expression for the time-evolution operator:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \frac{1}{n!} \int_{t_0}^t dt_1 \dots \int_{t_0}^t dt_n e^{-\epsilon(|t_1|+\dots+|t_n|)} T[\hat{V}_I(t_1) \dots \hat{V}_I(t_n)]$$

the numerator can be rewritten:

$$\begin{aligned} &\langle \phi_0 | \hat{U}_\epsilon(\infty, t) \hat{O}_I(t) \hat{U}_\epsilon(t, -\infty) | \phi_0 \rangle \\ &= \langle \phi_0 | \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \frac{1}{n!} \int_t^\infty dt_1 \dots \int_t^\infty dt_n T[\hat{V}_I(t_1) \dots \hat{V}_I(t_n)] \\ &\times e^{-\epsilon(|t_1|+\dots+|t_n|)} \hat{O}_I(t) \sum_{m=0}^{\infty} \left(-\frac{i}{\hbar} \right)^m \frac{1}{m!} \int_{-\infty}^t dt^1 \dots \int_{-\infty}^t dt^m \\ &\times e^{-\epsilon(|t^1|+\dots+|t^m|)} T[\hat{V}_I(t^1) \dots \hat{V}_I(t^m)] \\ &= \langle \phi_0 | \sum_{\nu=0}^{\infty} \left(-\frac{i}{\hbar} \right)^\nu \frac{1}{\nu!} \int_{-\infty}^\infty dt_1 \dots \int_{-\infty}^\infty dt_\nu e^{-\epsilon(|t_1|+\dots+|t_\nu|)} \\ &\times T[\hat{V}_I(t^1) \dots \hat{V}_I(t^\nu) \hat{O}_I(t)] | \phi_0 \rangle \end{aligned}$$

□

A.6 Mathematical induction proof of Wick's theorem

Theorem (Wick's theorem). $T[\phi(x_1) \dots \phi(x_m)] = N[\phi(x_1) \dots \phi(x_m) + \text{all possible contractions}]$

Proof. This proof is by induction on m , the number of fields. It was already shown that for $m = 2$:

$$T[\phi(x)\phi(y)] = N[\phi(x)\phi(y) + \overline{\phi(x)\phi(y)}]$$

With

$$\overline{\phi(x)\phi(y)} = \begin{cases} \{\phi^{(+)}(x), \phi^{(-)}(y)\} & \text{for } x^0 > y^0 \\ \{\phi^{(+)}(y), \phi^{(-)}(x)\} & \text{for } x^0 < y^0 \end{cases}$$

Now assuming the theorem is true for $m-1$ fields, it is necessary to prove it for m fields.

Without loss of generality, it can be assumed that $x_1^0 \geq x_2^0 \geq \dots \geq x_m^0$. Then, applying Wick's theorem to $\phi_2 \dots \phi_m$:

$$\begin{aligned} T[\phi_1 \dots \phi_m] &= \phi_1 N[\phi_2 \dots \phi_m \\ &\quad + \text{all possible contractions not involving } \phi_1] \\ &= (\phi_1^{(+)} + \phi_1^{(-)}) N[\phi_2 \dots \phi_m \\ &\quad + \text{all possible contractions not involving } \phi_1] \end{aligned}$$

The purpose is to move $\phi_1^{(+)}$ and $\phi_1^{(-)}$ inside the $N[\dots]$. $\phi_1^{(-)}$ can just be put inside since it is already in normal order. The $\phi_1^{(+)}$ must be anticommutated to the right past all the other ϕ 's.

$$\begin{aligned} \phi_1^{(+)} N[\phi_2 \dots \phi_m] &= N[\phi_2 \dots \phi_m] \phi_1^{(+)} + \{\phi_1^{(+)}, N[\phi_2 \dots \phi_m]\} \\ &= N[\phi_1^{(+)} \phi_2 \dots \phi_m] + N[\{\phi_1^{(+)}, \phi_2^{(-)}\} \phi_3 \dots \phi_m + \phi_2 \{\phi_1^{(+)}, \phi_3^{(-)}\} \phi_4 \dots \phi_m + \dots] \\ &= N[\phi_1^{(+)} \phi_2 \dots \phi_m + \overline{\phi_1 \phi_2} \phi_3 \dots \phi_m + \overline{\phi_1 \phi_2 \phi_3} \dots \phi_m + \dots] \end{aligned}$$

Then,

$$\begin{aligned} T[\phi_1 \dots \phi_m] &= N[\phi_1^{(-)} \phi_2 \dots \phi_m + \phi_1^{(+)} \phi_2 \dots \phi_m + \text{all possible contractions}] \\ &= N[\phi_1 \dots \phi_m + \text{all possible contractions}] \end{aligned}$$

□

A.7 Disconnected diagrams cancel out

(This section follows the proof given in reference [3], Chapter 4: "Interacting fields and Feynman diagrams", page 98)

A typical diagram for the numerator in equation 1.51 contains a piece connected to x and y and several disconnected pieces. Label the various possible disconnected pieces by V_i . The elements V_i are connected internally, but disconnected from external points.

Suppose that a diagram has n_i pieces of the form V_i for each i in addition to its one piece that is connected to x and y .

If we also let V_i denote the value of the piece V_i , then the value of such a diagram is:

$$(\text{value of connected piece}) \cdot \prod_i \frac{1}{n_i!} (V_i)^{n_i}$$

The $\frac{1}{n_i!}$ is the symmetry factor coming from interchanging the n_i copies of V_i .

The sum of all diagrams representing the numerator of the formula for the Green's function is then:

$$\sum_{\substack{\text{all} \\ \text{possible} \\ \text{connected} \\ \text{pieces}}} \sum_{\{n_i\}} (\text{value of connected piece}) \times \left(\prod_i \frac{1}{n_i!} (V_i)^{n_i} \right)$$

Where "all $\{n_i\}$ " means all ordered sets $\{n_1, n_2 \dots\}$ of non-negative integers.

The sum of the connected pieces factors out of this expression giving:

$$\text{Numerator} = \left(\sum \text{connected} \right) \times \sum_{\substack{\text{all} \\ \{n_i\}}} \left(\prod_i \frac{1}{n_i!} (V_i)^{n_i} \right) \quad (\text{A.52})$$

$$= \left(\sum \text{connected} \right) \times \left(\sum_{n_1} \frac{1}{n_1!} V_1^{n_1} \right) \left(\sum_{n_2} \frac{1}{n_2!} V_2^{n_2} \right) \dots \quad (\text{A.53})$$

$$= \left(\sum \text{connected} \right) \times \prod_i \left(\sum_{n_i} \frac{1}{n_i!} V_i^{n_i} \right) \quad (\text{A.54})$$

$$= \left(\sum \text{connected} \right) \times \prod_i \exp(V_i) \quad (\text{A.55})$$

$$= \left(\sum \text{connected} \right) \times \exp \left(\sum_i V_i \right) \quad (\text{A.56})$$

Therefore, the sum of all diagrams is equal to the sum of all connected diagrams times the exponential of the sum of all disconnected diagrams.

The denominator of formula 1.51, by an identical argument is the exponential of the sum of all disconnected diagrams which cancels the exponential of the disconnected diagrams in the numerator.

A.8 Proof of the generalized Wick's theorem

This proof follows the guidelines of reference [4].

Theorem (The generalized Wick's theorem). $Tr\{\hat{\rho}_0 T_\tau[\hat{A}\hat{B}\hat{C}\dots]\} =$ the sum over all possible fully contracted terms.

where \hat{A}, \hat{B}, \dots are field operators in the interaction picture.

Proof. Let $\varphi_j^0(\vec{x})$ be a single particle basis for the field operators:

$$\hat{\psi}(\vec{x}) = \sum_j \varphi_j^0(\vec{x}) \hat{a}_j \quad (\text{A.57})$$

$$\hat{\psi}^\dagger(\vec{x}) = \sum_j \varphi_j^0(\vec{x})^* \hat{a}_j^\dagger \quad (\text{A.58})$$

with:

$$k_0 \varphi_j^0(\vec{x}) = \underbrace{(\epsilon_j^0 - \mu)}_{=e_j} \varphi_j^0(\vec{x}) \quad (\text{A.59})$$

In the Interaction picture:

$$\hat{\psi}_I(\vec{x}\tau) = e^{\hat{K}_0\tau/\hbar} \sum_j \varphi_j^0(\vec{x}) \hat{a}_j e^{-\hat{K}_0\tau/\hbar} \quad (\text{A.60})$$

$$= \sum_j \varphi_j^0(\vec{x}) \hat{a}_j e^{-e_j\tau/\hbar} \quad (\text{A.61})$$

and

$$\hat{\psi}_I^\dagger(\vec{x}\tau) = \sum_j \varphi_j^0(\vec{x})^* \hat{a}_j^\dagger e^{e_j\tau/\hbar} \quad (\text{A.62})$$

To prove Wick's theorem first assume without loss of generality that the operators are already in the proper time order. The calculation will be easier if a general notation for an operator in the Interaction picture is introduced:

$$\hat{\psi}_I \quad \text{or} \quad \hat{\psi}_I^\dagger = \sum_j \eta_j(\vec{x}\tau) \hat{\alpha}_j$$

where

$$\hat{\alpha}_j = \hat{a}_j \quad \text{or} \quad \hat{a}_j^\dagger$$

and

$$\eta_j(\vec{x}\tau) = \varphi_j^0(\vec{x})e^{-e_j\tau/\hbar} \quad \text{or} \quad \varphi_j^0(\vec{x})^*e^{e_j\tau/\hbar}$$

With this notation, the l.h.s. of the equality in Wick's theorem becomes:

$$Tr \left\{ \hat{\rho}_0 \hat{A} \hat{B} \dots \hat{N} \right\} = \sum_a \sum_b \dots \sum_n \eta_a \eta_b \dots \eta_n Tr \left\{ \hat{\rho}_0 \hat{\alpha}_a \hat{\alpha}_b \dots \hat{\alpha}_n \right\} \quad (\text{A.63})$$

Anticommuting $\hat{\alpha}_a$ successively to the right:

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_a \hat{\alpha}_b \dots \hat{\alpha}_n \right\} &= Tr \left\{ \hat{\rho}_0 \{ \hat{\alpha}_a, \hat{\alpha}_b \} \hat{\alpha}_c \dots \hat{\alpha}_n \right\} \\ &- Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \{ \hat{\alpha}_a, \hat{\alpha}_c \} \dots \hat{\alpha}_n \right\} + Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \hat{\alpha}_c \dots \{ \hat{\alpha}_n, \hat{\alpha}_a \} \right\} \\ &- Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \hat{\alpha}_c \dots \hat{\alpha}_a \right\} \end{aligned}$$

The commutators are either 0 or 1 and may be taken outside the trace. Also:

$$e^{\beta \hat{K}_0} \hat{\alpha}_a e^{-\beta \hat{K}_0} = \hat{\alpha}_a e^{\pm \beta e_a} \quad (\text{A.64})$$

+ if $\hat{\alpha}_a$ is a creation operator, - if $\hat{\alpha}_a$ is an annihilation operator. Then,

$$\hat{\alpha}_a \hat{\rho}_0 = \hat{\rho}_0 \hat{\alpha}_a e^{\pm \beta e_a} \quad (\text{A.65})$$

So:

$$-Tr \left\{ \hat{\alpha}_a \hat{\rho}_0 \hat{\alpha}_b \dots \hat{\alpha}_n \right\} = -e^{\pm \beta e_a} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_a \hat{\alpha}_b \dots \hat{\alpha}_n \right\} \quad (\text{A.66})$$

and:

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_a \hat{\alpha}_b \dots \hat{\alpha}_n \right\} &= \frac{\{ \hat{\alpha}_a, \hat{\alpha}_b \}}{1 + e^{\pm \beta e_a}} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_c \dots \hat{\alpha}_n \right\} \\ &- \frac{\{ \hat{\alpha}_a, \hat{\alpha}_c \}}{1 + e^{\pm \beta e_a}} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \dots \hat{\alpha}_n \right\} + \dots + \frac{\{ \hat{\alpha}_a, \hat{\alpha}_n \}}{1 + e^{\pm \beta e_a}} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \dots \hat{\alpha}_{n-1} \right\} \end{aligned} \quad (\text{A.67})$$

Define a contraction as:

$$\overline{\hat{\alpha}_a \hat{\alpha}_b} = \frac{\{ \hat{\alpha}_a, \hat{\alpha}_b \}}{1 + e^{\pm \beta e_a}} \quad (\text{A.68})$$

This definition is equivalent to the definition in equation 1.134. Then,

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_a \hat{\alpha}_b \dots \hat{\alpha}_n \right\} &= \overline{\hat{\alpha}_a \hat{\alpha}_b} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_c \dots \hat{\alpha}_n \right\} \\ &- \overline{\hat{\alpha}_a \hat{\alpha}_c} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \dots \hat{\alpha}_n \right\} + \dots + \overline{\hat{\alpha}_a \hat{\alpha}_n} Tr \left\{ \hat{\rho}_0 \hat{\alpha}_b \dots \hat{\alpha}_{n-1} \right\} \\ &= Tr \left\{ \hat{\rho}_0 \overline{\hat{\alpha}_a \hat{\alpha}_b} \hat{\alpha}_c \dots \hat{\alpha}_n \right\} + Tr \left\{ \hat{\rho}_0 \overline{\hat{\alpha}_a \hat{\alpha}_c} \hat{\alpha}_b \dots \hat{\alpha}_n \right\} \\ &\quad + \dots + Tr \left\{ \hat{\rho}_0 \overline{\hat{\alpha}_a \hat{\alpha}_n} \hat{\alpha}_b \dots \hat{\alpha}_n \right\} \end{aligned}$$

Going back to the field operators:

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \hat{A} \hat{B} \hat{C} \dots \hat{N} \right\} &= Tr \left\{ \hat{\rho}_0 \overline{\hat{A} \hat{B}} \hat{C} \dots \hat{N} \right\} \\ &+ Tr \left\{ \hat{\rho}_0 \overline{\hat{A} \hat{C}} \hat{B} \dots \hat{N} \right\} + \dots + Tr \left\{ \hat{\rho}_0 \overline{\hat{A} \hat{N}} \hat{B} \dots \hat{N} \right\} \end{aligned}$$

The contraction is a number and may be taken out of the trace leaving a structure of the same kind as the one originally considered. By repeating the algorithm in the end the result will be:

$$Tr \left\{ \hat{\rho}_0 \hat{A} \hat{B} \hat{C} \dots \hat{N} \right\} = \text{sum of all possible fully contracted terms}$$

□

A.9 Functional derivatives of expectation values of operators

Consider a perturbation $\delta\hat{V}(t)$ in the Hamiltonian. Taking the variation of the equations for the time evolution operator \hat{U} :

$$\begin{aligned} i\partial_t\hat{U}(t,t') &= \hat{H}(t)\hat{U}(t,t') \\ i\partial_{t'}\hat{U}(t,t') &= -\hat{U}(t,t')\hat{H}(t') \\ \hat{U}(t,t) &= 1 \end{aligned}$$

will result in the following equations:

$$i\partial_t\delta\hat{U}(t,t') = \delta\hat{V}(t)\hat{U}(t,t') + \hat{H}(t)\delta\hat{U}(t,t') \quad (\text{A.69})$$

$$i\partial_{t'}\delta\hat{U}(t,t') = -\hat{U}(t,t')\delta\hat{V}(t') - \delta\hat{U}(t,t')\hat{H}(t') \quad (\text{A.70})$$

$$\delta\hat{U}(t,t) = 0 \quad (\text{A.71})$$

A solution looks like this:

$$\delta\hat{U}(t,t') = -i \int_{t'}^t d\tau \hat{U}(t,\tau)\delta\hat{V}(\tau)\hat{U}(\tau,t') \quad (\text{A.72})$$

Checking this solution:

$$\begin{aligned} \partial_t \int_{t'}^t d\tau \hat{U}(t,\tau)\delta\hat{V}(\tau)\hat{U}(\tau,t') &= \int_{t'}^t d\tau \partial_t \hat{U}(t,\tau)\delta\hat{V}(\tau)\hat{U}(\tau,t') + \delta\hat{V}(t)\hat{U}(t,t') \\ &= \delta\hat{V}(t)\hat{U}(t,t') + \hat{H}(t)\delta\hat{U}(t,t') \end{aligned}$$

If $\delta\hat{V}(t) = \int d\vec{x}\delta v(\vec{x}t)\hat{n}(\vec{x})$ then:

$$\begin{aligned} \frac{\delta\hat{U}(t_0 - i\beta, t_0)}{\delta v(\vec{x}t)} &= -i \frac{\delta}{\delta v(\vec{x}t)} \left(\int_{t_0}^{t_0 - i\beta} d\tau \hat{U}(t_0 - i\beta, \tau) \int d\vec{x}\delta v(\vec{x}t)\hat{n}(\vec{x})\hat{U}(\tau, t_0) \right) \\ &= -i\hat{U}(t_0 - i\beta, t_0)\hat{n}(\vec{x})\hat{U}(t_0, t_0) \\ &= -i\hat{U}(t_0 - i\beta, t_0)\hat{n}_H(\vec{x}t) \end{aligned} \quad (\text{A.73})$$

Now, calculate the change in the expectation value of an operator:

$$\begin{aligned} \frac{\delta\langle\hat{O}(t_1)\rangle}{\delta v(\vec{x}_2t_2)} &= \frac{\delta}{\delta v(\vec{x}_2t_2)} \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t_1)\hat{O}\hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &= \frac{\frac{\delta}{\delta v(\vec{x}_2t_2)} \text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t_1)\hat{O}\hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\ &\quad - \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t_1)\hat{O}\hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}^2} \\ &= \frac{\delta \text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}{\delta v(\vec{x}_2t_2)} \cdot \frac{1}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \end{aligned}$$

And further:

$$\begin{aligned}
\frac{\delta\langle\hat{O}(t_1)\rangle}{\delta v(\vec{x}_2 t_2)} &= \theta(t_1, t_2) \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_1) \hat{O} \frac{\delta\hat{U}(t_1, t_0)}{\delta v(\vec{x}_2 t_2)} \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&+ \theta(t_2, t_1) \frac{\text{Tr} \left\{ \frac{\delta\hat{U}(t_0 - i\beta, t_1)}{\delta v(\vec{x}_2 t_2)} \hat{O} \hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&- \langle\hat{O}(t_1)\rangle \cdot \frac{\delta\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}{\delta v(\vec{x}_2 t_2)} \cdot \frac{1}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= -i\theta(t_1, t_2) \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_1) \hat{O} \hat{U}(t_1, t_2) \hat{n}(\vec{x}_2) \hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&- i\theta(t_2, t_1) \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2) \hat{n}(\vec{x}_2) \hat{U}(t_2, t_1) \hat{O} \hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&+ i\langle\hat{O}(t_1)\rangle \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2) \hat{n}(\vec{x}_2) \hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= -i\theta(t_1, t_2) \langle\hat{O}(t_1) \hat{n}(\vec{x}_2 t_2)\rangle - i\theta(t_2, t_1) \langle\hat{n}(\vec{x}_2 t_2) \hat{O}(t_1)\rangle \tag{A.74} \\
&+ i\langle\hat{O}(t_1)\rangle \langle\hat{n}(\vec{x}_2 t_2)\rangle \tag{A.75}
\end{aligned}$$

Similarly, for the functional derivative of a time-ordered product:

$$\frac{\delta\langle T_c[\hat{A}(t_1) \hat{B}(t_2)]\rangle}{\delta v(\vec{x}_3 t_3)} = -i\langle T_c[\hat{A}(t_1) \hat{B}(t_2) \hat{n}(\vec{x}_3 t_3)]\rangle + i\langle\hat{n}(\vec{x}_3 t_3)\rangle \langle T_c[\hat{A}(t_1) \hat{B}(t_2)]\rangle \tag{A.76}$$

Therefore,

$$\frac{\delta G(1, 2)}{\delta v(3)} = -i \frac{\delta}{\delta v(3)} \langle T_c[\hat{\psi}_H(1) \psi_H^\dagger(2)]\rangle \tag{A.77}$$

$$= -\langle T_c[\hat{\psi}_H(1) \psi_H^\dagger(2) \hat{n}_H(3)]\rangle + \langle\hat{n}_H(3)\rangle \langle T_c[\hat{\psi}_H(1) \psi_H^\dagger(2)]\rangle \tag{A.78}$$

A.10 The Kubo-Martin-Schwinger boundary conditions

$$\begin{aligned}
G(x_1 t_0 - i\beta, 2) &= -i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t_0 - i\beta) \hat{\psi}(\vec{x}_1) \hat{U}(t_0 - i\beta, t_2) \hat{\psi}^\dagger(\vec{x}_2) \hat{U}(t_2, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= -i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_2) \hat{\psi}^\dagger(\vec{x}_2) \hat{U}(t_2, t_0) \hat{\psi}(\vec{x}_1) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= -i \langle \hat{\psi}_H^\dagger(\vec{x}_2 t_2) \hat{\psi}_H(\vec{x}_1 t_0) \rangle \\
&= i \langle \hat{\psi}_H(\vec{x}_1 t_0) \hat{\psi}_H^\dagger(2) \rangle \\
&= -G(\vec{x}_1 t_0, 2) \tag{A.79}
\end{aligned}$$

Also,

$$\begin{aligned}
G(1, \vec{x}_2 t_0 - i\beta) &= i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t_0 - i\beta) \hat{\psi}^\dagger(\vec{x}_2) \hat{U}(t_0 - i\beta, t_1) \hat{\psi}(\vec{x}_1) \hat{U}(t_1, t_0) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= i \frac{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t_1) \hat{\psi}(\vec{x}_1) \hat{U}(t_1, t_0) \hat{\psi}^\dagger(\vec{x}_2) \right\}}{\text{Tr} \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} \\
&= i \langle T_c [\hat{\psi}(1) \hat{\psi}^\dagger(\vec{x}_2 t_0)] \rangle \\
&= -G(1, \vec{x}_2 t_0)
\end{aligned} \tag{A.80}$$

Next, it is straightforward to check that a general solution to the equation:

$$(i\partial_{t_1} - \hat{h}(1)) \frac{\delta G(1, 1')}{\delta v(2)} - \int d^3\Sigma(1, 3) \frac{\delta G(3, 1)}{\delta v(2)} = \delta(1, 2) G(1, 1') + \int d^3 \frac{\delta \Sigma(1, 3)}{\delta v(2)} G(3, 1') \tag{A.81}$$

is:

$$\frac{\delta G(1, 1')}{\delta v(2)} = G(1, 2) G(2, 1') + \int d^3 d^4 G(1, 3) \frac{\delta \Sigma(3, 4)}{\delta v(2)} G(4, 1') + C(1, 1', 2) \tag{A.82}$$

where C is a solution of the equation:

$$(i\partial_{t_1} - \hat{h}(1)) C(1, 1', 2) - \int d^3 \Sigma(1, 3) C(3, 1', 2) = 0 \tag{A.83}$$

Then C must also obey the Martin-Schwinger boundary conditions:

$$C(\vec{x}_1 t_0 - i\beta, 1') = -C(\vec{x}_1 t_0, 1') \tag{A.84}$$

$C = 0$ satisfies both the homogeneous equation and the boundary conditions therefore it is uniquely fixed.

A.11 Keldysh book-keeping

This appendix contains examples of calculations with contour-ordered functions following the guidelines in references [1] and [8].

Consider two functions a and b of the form:

$$a(t, t') = a^\delta(t) \delta(t, t') + \theta(t, t') a^>(t, t') + \theta(t', t) a^<(t, t') \tag{A.85}$$

The aim is to calculate contour integrals of the product of the two functions:

$$c(t, t') = \int_c d\bar{t} a(t, \bar{t}) b(\bar{t}, t') \tag{A.86}$$

Replacing the expressions for a and b will result in the general expression for c:

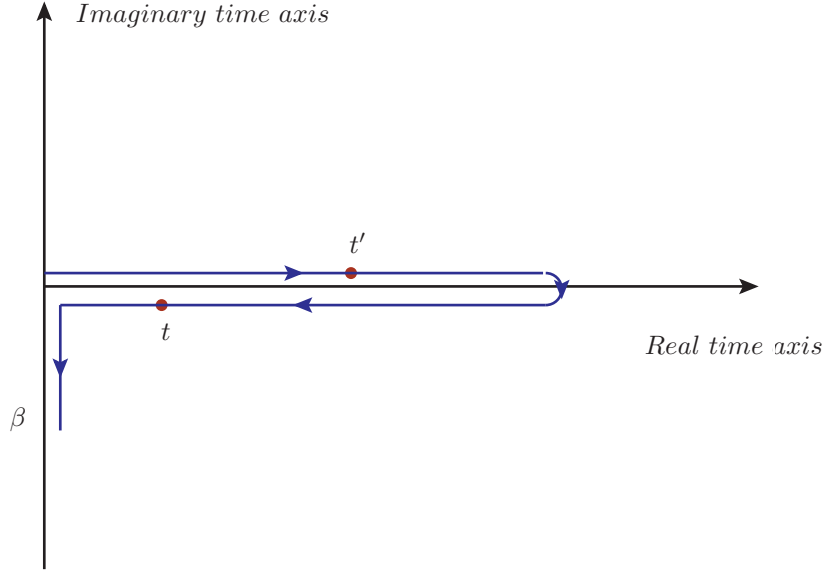
$$c(t, t') = a^\delta(t) b(t, t') + a(t, t') b^\delta(t') \tag{A.87}$$

$$+ \int_c d\bar{t} (\theta(t, \bar{t}) \theta(\bar{t}, t') a^>(t, \bar{t}) b^>(\bar{t}, t') + \theta(t, \bar{t}) \theta(t', \bar{t}) a^>(t, \bar{t}) b^<(\bar{t}, t')) \tag{A.88}$$

$$+ \theta(\bar{t}, t) \theta(\bar{t}, t') a^<(t, \bar{t}) b^>(\bar{t}, t') + \theta(\bar{t}, t) \theta(t', \bar{t}) a^<(t, \bar{t}) b^<(\bar{t}, t')) \tag{A.89}$$

Now let's see how c looks for different positions of t and t' on the contour.

For example, for $t > t'$ and both on the real part of the contour:



$$c^>(t, t') = a^\delta(t)b^>(t, t') + a^>(t, t')b^\delta(t') \quad (\text{A.90})$$

$$+ \int_{t'}^t d\bar{t} a^>(t, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^{t'} d\bar{t} a^>(t, \bar{t})b^<(\bar{t}, t') + \int_t^{t_0-i\beta} d\bar{t} a^<(t, \bar{t})b^>(\bar{t}, t') \quad (\text{A.91})$$

Denoting:

$$a^<(t, t_0 - i\tau) = a^\lceil(t, \tau) \quad (\text{A.92})$$

$$a^>(t_0 - i\tau, t) = a^\lrcorner(\tau, t) \quad (\text{A.93})$$

$$c^>(t, t') = a^\delta(t)b^>(t, t') + a^>(t, t')b^\delta(t') \quad (\text{A.94})$$

$$+ \int_{t_0}^t d\bar{t} a^>(t, \bar{t})b^>(\bar{t}, t') - \int_{t_0}^{t'} d\bar{t} a^>(t, \bar{t})(b^>(\bar{t}, t') - b^<(\bar{t}, t')) \quad (\text{A.95})$$

$$- \int_{t_0}^t d\bar{t} a^<(t, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^{t_0-i\beta} d\bar{t} a^<(t, \bar{t})b^>(\bar{t}, t') \quad (\text{A.96})$$

Define the retarded and advanced functions in physical time:

$$a^R(t, t') = a^\delta(t)\delta(t - t') + \theta(t, t')(a^>(t, t') - a^<(t, t')) \quad (\text{A.97})$$

$$a^A(t, t') = a^\delta(t)\delta(t - t') - \theta(t', t)(a^>(t, t') - a^<(t, t')) \quad (\text{A.98})$$

Thus,

$$\begin{aligned} c^>(t, t') &= \int_{t_0}^{\infty} d\bar{t} ((a^\delta(\bar{t})\delta(\bar{t} - t) + \theta(t, \bar{t})(a^>(t, \bar{t}) - a^<(t, \bar{t})))b^>(\bar{t}, t')) \\ &+ \int_{t_0}^{\infty} d\bar{t} a^>(t, \bar{t})(b^\delta(\bar{t})\delta(\bar{t} - t') - \theta(t', \bar{t})(b^>(\bar{t}, t') - b^<(\bar{t}, t'))) - i \int_0^\beta d\tau a^\lceil(t, \tau)b^\lrcorner(\tau, t') \\ &= \int_{t_0}^{\infty} d\bar{t} a^R(t, \bar{t})b^>(\bar{t}, t') + \int_{t_0}^{\infty} d\bar{t} a^>(t, \bar{t})b^A(\bar{t}, t') - i \int_0^\beta d\tau a^\lceil(t, \tau)b^\lrcorner(\tau, t') \end{aligned} \quad (\text{A.99})$$

Introducing notations:

$$a \cdot b = \int_{t_0}^{\infty} d\bar{t} a(\bar{t})b(\bar{t}) \quad (\text{A.100})$$

$$a \star b = -i \int_0^\beta d\tau a(\tau) b(\tau) \quad (\text{A.101})$$

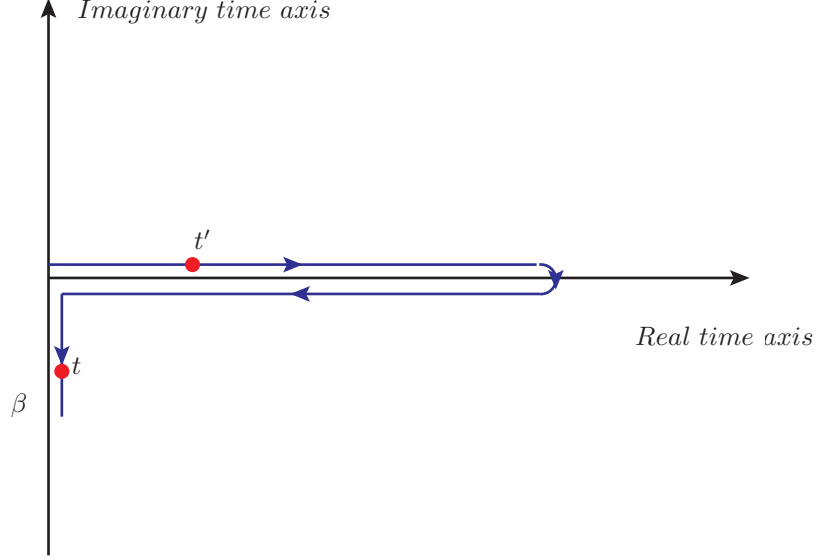
allows one to write in a short form the expression for $c^>$:

$$c^> = a^R \cdot b^> + a^> \cdot b^A + a^\lceil \star b^\lceil \quad (\text{A.102})$$

Analogously,

$$c^< = a^R \cdot b^< + a^< \cdot b^A + a^\lceil \star b^\lceil \quad (\text{A.103})$$

Now for a different position of t and t' :



$$\begin{aligned}
c^>(t_0 - i\tau, t') &= c^\lceil(\tau, t') = a^\delta(t_0 - i\tau) b^>(t_0 - i\tau, t') \\
&+ a^>(t_0 - i\tau, t') b^\delta(t') + \int_{t'}^{t_0 - i\tau} d\bar{t} a^>(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') \\
&+ \int_{t_0}^{t'} d\bar{t} a^>(t_0 - i\tau, \bar{t}) b^<(\bar{t}, t') + \int_{t_0 - i\tau}^{t_0 - i\beta} d\bar{t} a^<(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') \\
&= a^\lceil(\tau, t') b^\delta(t') + a^\delta(t_0 - i\tau) b^\lceil(\tau, t') - \int_{t_0}^{t'} d\bar{t} a^\lceil(\tau, \bar{t}) (b^>(\bar{t}, t') - b^<(\bar{t}, t')) \\
&+ \int_{t_0}^{t_0 - i\tau} d\bar{t} a^>(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') + \int_{t_0 - i\tau}^{t_0 - i\beta} d\bar{t} a^<(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') \\
&= \int_{t_0}^{\infty} d\bar{t} a^\lceil(\tau, \bar{t}) (b^\delta(t') \delta(\bar{t} - t') - \theta(t', \bar{t}) (b^>(\bar{t}, t') - b^<(\bar{t}, t'))) + a^\delta(t_0 - i\tau) b^\lceil(\tau, t') \\
&+ \int_{t_0}^{t_0 - i\tau} d\bar{t} a^>(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') + \int_{t_0 - i\tau}^{t_0 - i\beta} d\bar{t} a^<(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t') \\
&= \int_{t_0}^{\infty} d\bar{t} a^\lceil(\tau, \bar{t}) b^A(\bar{t}, t') + \int_0^\beta d\bar{\tau} a^\delta(t_0 - i\bar{\tau}) b^\lceil(\bar{\tau}, t') \delta(\bar{\tau}, \tau) \\
&+ \int_{t_0}^{t_0 - i\beta} d\bar{t} (\theta(t_0 - i\tau, \bar{t}) a^>(t_0 - i\tau, \bar{t}) + \theta(\bar{t}, t_0 - i\tau) a^<(t_0 - i\tau, \bar{t}) b^>(\bar{t}, t')) \quad (\text{A.104})
\end{aligned}$$

Making the change of variables: $\bar{t} = t_0 - i\bar{\tau}$ and defining the Matsubara function a^M as the function a restricted to the imaginary part of the contour:

$$a^M(\tau, \bar{\tau}) = ia^\delta(\bar{\tau}) \delta(\tau - \bar{\tau}) + \theta(\tau, \bar{\tau}) a^>(\tau, \bar{\tau}) + \theta(\bar{\tau}, \tau) a^<(\tau, \bar{\tau}) \quad (\text{A.105})$$

yields:

$$c^\lceil(\tau, t') = \int_{t_0}^{\infty} d\bar{t} a^\lceil(\tau, \bar{t}) b^A(\bar{t}, t') - i \int_0^{\beta} d\bar{\tau} a^M(\tau, \bar{\tau}) b^\lceil(\bar{\tau}, t') d\bar{\tau} \quad (\text{A.106})$$

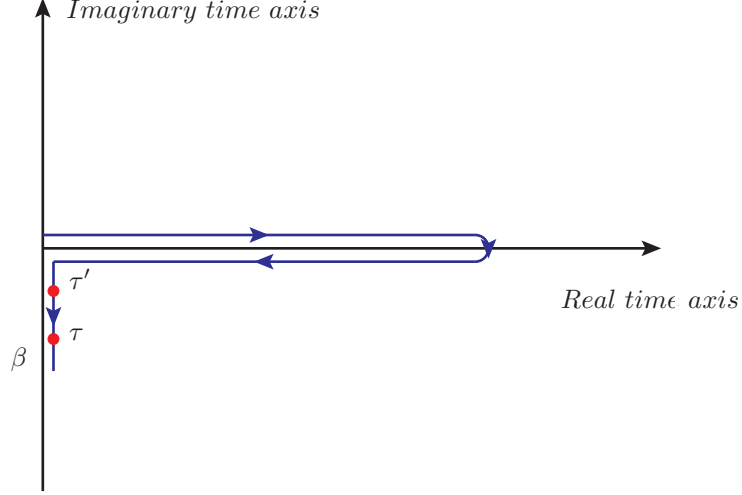
and in short notation:

$$c^\lceil = a^\lceil \cdot b^A + a^M \star b^\lceil \quad (\text{A.107})$$

Analogously,

$$c^\lrcorner = a^R \cdot b^\lrcorner + a^\lrcorner \star b^M \quad (\text{A.108})$$

Finally when both arguments of c are on the imaginary part of the contour:



$$c^M = a^M \star b^M \quad (\text{A.109})$$

Next, these results will be applied to the equations:

$$(i\partial_{t_1} - \hat{h}(1))G(1, 2) = \delta(1, 2) + \int_c d^3\Sigma(1, 3)G(3, 2) \quad (\text{A.110})$$

$$(-i\partial_{t_2} - \hat{h}(2))G(1, 2) = \delta(1, 2) + \int_c d^3G(1, 3)\Sigma(3, 2) \quad (\text{A.111})$$

to yield the Kadanoff-Baym equations:

$$(i\partial_{t_1} - \hat{h}(1))G^{\lessgtr}(1, 2) = (\Sigma^R \cdot G^{\lessgtr} + \Sigma^{\lessgtr} \cdot G^A + \Sigma^\lceil \star G^\lceil)(1, 2) \quad (\text{A.112})$$

$$(-i\partial_{t_2} - \hat{h}(2))G^{\lessgtr}(1, 2) = (G^R \cdot \Sigma^{\lessgtr} + G^{\lessgtr} \cdot \Sigma^A + G^\lceil \star \Sigma^\lceil)(1, 2) \quad (\text{A.113})$$

$$(i\partial_{t_1} - \hat{h}(1))G^\lceil(1, 2) = (\Sigma^R \cdot G^\lceil + \Sigma^\lceil \star G^M)(1, 2) \quad (\text{A.114})$$

$$(i\partial_{t_1} - \hat{h}(1))G^\lrcorner(1, 2) = (\Sigma^\lceil \cdot G^A + \Sigma^M \star G^\lrcorner)(1, 2) \quad (\text{A.115})$$

$$(-i\partial_{t_2} - \hat{h}(2))G^\lceil(1, 2) = (G^A \cdot \Sigma^\lceil + G^\lceil \star \Sigma^M)(1, 2) \quad (\text{A.116})$$

$$(-i\partial_{t_2} - \hat{h}(2))G^\lrcorner(1, 2) = (G^\lrcorner \cdot \Sigma^A + G^M \star \Sigma^\lrcorner)(1, 2) \quad (\text{A.117})$$

$$(i\partial_{t_1} - \hat{h}(1))G^M(1, 2) = i\delta(\tau_1 - \tau_2) + (\Sigma^M \star G^M)(1, 2) \quad (\text{A.118})$$

$$(-i\partial_{t_2} - \hat{h}(2))G^M(1, 2) = i\delta(\tau_1 - \tau_2) + (G^M \star \Sigma^M)(1, 2) \quad (\text{A.119})$$

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