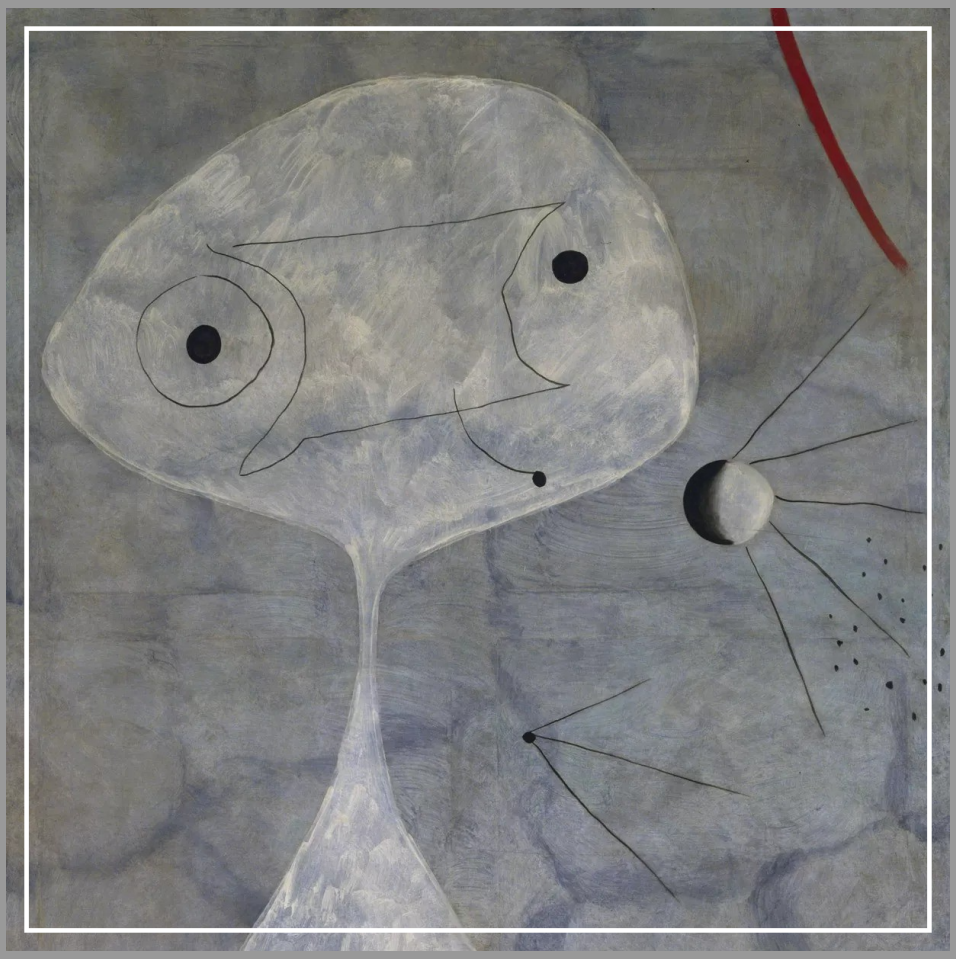
Journal notes on:

Introduction to Green's function formalism

by Francisco Lobo



CONTENTS

ACKNOWLEDGMENTS

Given their nature as personal journal notes, these sections remain perpetually incomplete and are subject to ongoing revision. While you are more than welcome to read them, please be advised that they may contain errors or misinterpretations on my part. If your expertise or intuition suggests that something appears inaccurate or questionable, your assessment is likely correct. Should you identify any such issues, I would be deeply grateful if you could contact me regarding the matter, as this would allow me to make corrections and further my understanding.

Alongside these personal journal notes, an accompanying worksheet is provided. Given that the notes primarily emphasize physical intuition and conceptual depth rather than rigorous mathematical derivations, lengthier or more tedious calculations have been separated into this supplementary material to maintain clarity and focus in the main text. These exercises are referenced at relevant points, particularly following claims that may appear mathematically abrupt. If a result seems unclear at first glance, the reader may consult the exercise sheet for a complete derivation. These exercises largely constitute "do once in a lifetime" endeavors, as their derivations hold no hidden complexity upon inspection. Having demystified them, one may thereafter accept the results without repeating the process. As another supplementary material, there is a GitHub repository at https://github.com/franciscolobo1880/topoSC where you can check the code that generate the figures of the various models. This is done in *Julia* using the *Quantica.jl* package by Pablo San-Jose, my PhD advisor. Check *Quantica.jl*'s repository and it's tutorial at https://github.com/pablosanjose/Quantica.jl.

I would like to express my sincere gratitude to my advisors, Pablo San-Jose and Elsa Prada, for their invaluable guidance, support, and mentorship throughout the course of my thesis. Their broad expertise has been instrumental in the development of this book, especially considering that many of its core topics first emerged as recurring themes I encountered during our thesis meetings. In particular, Elsa Prada's presentation on Topological Insulators and Superconductors served as a key inspiration and provided the initial conceptual framework from which this book began to take shape.

I am also deeply grateful to my colleagues, César Robles and Carlos Paya, as well as to my good friend, Tiago Antão, for their assistance and for the many stimulating and insightful discussions we shared. Their input has significantly contributed to the refinement of my ideas and the overall coherence of this work.

My personal website, which includes all my research papers as well as journal notes on various topics, such as "Introduction to topological superconductivity", can be found at https://franciscolobo1880.github.io/.

PREFACE

The preface first paragraph will be written once I have a good idea of what these notes will look like conceptually. The following paragraphs, the ones actually describing the contents of this book will be written when the book is mostly finished.

Part I
Introduction to Green's functions formalism

I. INTRODUCTION

A. Forewords to linear response theory

1. The density matrix

Consider an ensemble consisting of many ($N \gg 1$) identically prepared systems, all of which are characterized by a Hamiltonian H that may be dependent on time. Let $\left|\psi^{(n)}\right\rangle$ be the time-dependent normalized wave function corresponding to the nth system in this ensemble. The time-dependent Schrödinger equation can be written as

$$i\frac{d}{dt}\left|\psi^{(n)}\right\rangle = H\left|\psi^{(n)}\right\rangle, \text{ with } n = 1, 2, ..., N \tag{1}$$

Moreover, consider the complete set of orthonormal functions $|\alpha\rangle$, so that the wave functions at any time t can be expanded as

$$\left|\psi^{(n)}\right\rangle = \sum_{\alpha} C_{\alpha}^{(n)}(t)\,|\alpha\rangle \tag{2}$$

with the time-dependent coefficients $C_{\alpha}^{(n)}(t)$, being the probability of finding the nth system in the states $|\alpha\rangle$ at a time t, satisfying $C_{\alpha}^{(n)}(t) = \langle\alpha|\psi^{(n)}\rangle$ and, being a complete and orthogonal set, $\sum_{\alpha}\left|C_{\alpha}^{(n)}(t)\right|^2 = 1$. Hence, each nth state of the system in the ensemble can be described in terms of the set of coefficients $\left\{C_{\alpha}^{(n)}(t)\right\}$ for different α. It follows that

$$i\frac{d}{dt}C_{\alpha}^{(n)}(t) = \sum_{\beta}\langle\alpha|\,H\,|\beta\rangle\,C_{\beta}^{(n)}(t) \tag{3}$$

The density matrix of the system, denoted by ρ, is then defined as the operator with matrix elements given by

$$\rho_{\alpha\beta} = \frac{1}{\mathcal{N}}\sum_{n=1}^{N} C_{\beta}^{(n)}(t)\left\{C_{\alpha}^{(n)}(t)\right\}^{*}, \tag{4}$$

meaning that the (α, β) matrix element of ρ is the ensemble average of the "probabilities" $C_{\beta}^{(n)}(t)\left\{C_{\alpha}^{(n)}(t)\right\}^{*}$. In particular, see that the diagonal elements $\rho_{\alpha\alpha}$ are the ensemble average of the actual probability $\left|C_{\alpha}^{(n)}(t)\right|^2$ of the system being at the state $|\alpha\rangle$. Because the probabilities add to give unity, it follows that $\mathrm{Tr}(\rho) = 1$. Another most important notion is that is satisfies $id/dt\rho = [H, \rho]$.

2. Thermal equilibrium

On one hand, from the definition of the mean value of some operator O and from what we gathered from the analysis above we have that

$$\langle O\rangle = \frac{1}{N}\sum_{n=1}^{N}\left\langle\psi^{(n)}\right|H\left|\psi^{(n)}\right\rangle = \mathrm{Tr}(\rho O). \tag{5}$$

One the other hand, from statistical physics we know that the equilibrium thermal average in a grand canonical ensemble is given by

$$\langle O\rangle = \frac{1}{Z}\sum_{\alpha}\langle\alpha|\,O\,|\alpha\rangle\, e^{-\beta_B(\varepsilon_\alpha-\mu N_\alpha)} = \frac{1}{Z}\mathrm{Tr}\left(Oe^{-\beta_B(H-\mu\mathcal{N})}\right) \tag{6}$$
$$\text{with } Z = \sum_{\alpha} e^{-\beta_B(\varepsilon_\alpha-\mu N_\alpha)} = \mathrm{Tr}\left(e^{-\beta_B(H-\mu\mathcal{N})}\right)$$

the grand partition function, $\beta_B = 1/k_BT$ the Boltzmann temperature and ε_α the energy and N_α the number of particles of the state $|\alpha\rangle$. For the second equality H denotes the system's Hamiltonian and $\mathcal{N}$ the number operator. Putting the two together we get that

$$\rho = \frac{1}{Z}\mathrm{Tr}e^{-\beta_B(H-\mu\mathcal{N})}. \tag{7}$$

This equation will not, of course, apply in a non-equilibrium situation.

3. *Response function*

Consider a system, otherwise unperturbed and in equilibrium, which is perturbed by a small time-varying external force. Let

$$H = H_0 + H_1$$

be the total Hamiltonian with H_0 describing the unperturbed system and $H_1 = -Bf(t)$ describing the time-dependent perturbation, with B a QM operator and $f(t)$ is a scalar function that describes the time dependence of the interaction. In the same note, the system's density matrix reads $\rho = \rho_0 + \rho_1$. Moreover, as a boundary condition, we assume that at $t \to -\infty$ the system is in equilibrium and unperturbed such that $\rho_1 \to 0$ and $H_1 \to 0$. The density matrix equation of motion reads

$$i\frac{d\rho}{dt} = [H_0,\rho_0] + [H_0,\rho_1] + [H_1,\rho_0] + [H_1,\rho_1] \Leftrightarrow i\frac{d\rho_1}{dt} \approx [H_0,\rho_1] + [H_1,\rho_0] \tag{8}$$

$$\Rightarrow \rho_1 = -i\int_{-\infty}^{t} dt' e^{iH_0(t'-t)}\,[H_1,\rho_0]\,e^{-iH_0(t'-t)} \tag{9}$$

where $[H_0,\rho_0] = 0$ by definition and $[H_1,\rho_1]$ is neglected because it is of second order in the small quantities H_1 and ρ_1. By direct substitution and some clever manipulation (see exercise.IV.x), the time-dependent average of a given operator A given by $\langle A\rangle = \mathrm{Tr}(\rho A) = \mathrm{Tr}(\rho_0 A) + \mathrm{Tr}(\rho_1 A)$, or rather $\langle A\rangle = \langle A\rangle_0 + \langle A\rangle_1$, will follow as

$$\langle A\rangle_1 = -i\int_{-\infty}^{t} dt'\,\langle[A,H_1(t'-t)]\rangle_0 = -i\int_{-\infty}^{t} dt'\,\langle[A,B(t'-t)]\rangle_0\, f(t') \tag{10}$$

This result tells us that to calculate an average $\langle A\rangle$ for a non-equilibrium system at time t we may instead calculate a different average, namely the correlation function $\langle[A,B(t'-t)]\rangle_0$, which is for the unperturbed system.

Hint to retarded GFs as a response function

As foreshadowing and motivation of what's to come, we will eventually understand that the preceding linear response result can be re-expressed as

$$\langle A\rangle_1 = -\int_{-\infty}^{+\infty} dt' G^R(A;B|t-t')f(t') \tag{11}$$

with $G^R(A;B|t-t')$ being the so-called *retarded* Green's functions which, in this context, can then be thought as a "response function.". See that, if the perturbing force were to be an abrupt impulsive in time applied at $t'=0$ such that $f(t)=\delta(t)$, we would obtain directly that $\langle A\rangle_1 = -G^R(A;B|t)$. This result is reminiscent of the role of the classical GFs, bridging a direct interpretation that the GF describes the behavior of the system in the presence of an abrupt perturbation. Moreover, see that the above expression is just a convolution in time domain between two functions in frequency domain; a perturbation $f(\omega)$ is applied to the system and it responds in through the GF $G^R(A;B|\omega)$. Further ahead we will see concrete examples of this notion, for example, in the context of the magnetic susceptibility and the dielectric response function of an electron gas.

B. Survey of classical Green's functions

Let us consider the following linear differential equation

$$\mathcal{L}x(t) - \lambda x(t) = f(t)$$

with $\mathcal{L}$ some Hermitian differential operator, usually a linear combination of terms involving powers of d/dt, ω_0 a constant and $f(t)$ an inhomogeneous term. This could, for example, describe some type of one-dimensional damped harmonic oscillator motion if $\mathcal{L} = d_t^2 + \Gamma d_t$ with Γ the damping ration, λ its undamped frequency and $f(t)$ an external perturbative force. In general, initial value boundary conditions would also be specified. Also, in the absence of $f(x)$ we would have a homogeneous eigenvalue equation.

A common procedure used to solve this equation involves expanding both $x(t)$ and $f(x)$ in terms of the eigenfunctions $x_n(t)$ with $n=1,2,3,...$, of the operator $\mathcal{L}$, this is,

$$x(t) = \sum_n \alpha_n x_n(t) \text{ and } f(t) = \sum_n \beta_n x_n(t) \tag{12}$$

with α_n and β_n coefficients to be determined. The connection between these coefficients can simply be obtained by substituting the previously mentioned expressions into the linear differential equation and using the orthogonality properties of the eigenfunction. In this way it can be deduced that

$$x(t) = \sum_n \frac{\beta_n x_n(t)}{\lambda_n - \lambda} \tag{13}$$

with λ_n the eigenvalue corresponding to eigenfunction $x_n(t)$. Then, by utilizing the inverse expansions to those in Eq.(12), the preceding result can be rewritten (see exercise) as

$$x(t) = \int dt' G(t,t') f(t') \text{ with } G(t,t') = \sum_n \frac{x_n(t) x_n^*(t')}{\lambda_n - \lambda}$$

the so-called classical Green's function of the system. The preceding results hold quite generally for any $f(t)$.

Let us now take the inhomogeneous term to be a delta function at the origin $\delta(t=0)$. Directly from the above expression we have that $x(t) = \int dt' G(t,t')\delta(t') = G(t,0)$. If follows that the classical GF solution can be obtained by solving instead $(\mathcal{L}-\lambda)G(t,t') = \delta(t-t')$. This preceding result nicely illustrates a physical interpretation of the classical GF. It represents the solution (as a function of t) for the differential equation when the source term has the form of an impulse, i.e $f(t)=\delta(t)$.

II. TIME-DEPENDENT PERTURBATION THEORY

A. S-matrix in the interaction picture

Consider a system with dynamics governed by the time-dependent Hamiltonian

$$H(t) = H_0 + V(t) + H_{\text{int}} \tag{14}$$

with H_0 a single-particle term in thermal equilibrium, $V(t)$ a single-particle term that depends on time and was turned on at a given time $t' = t_0$, and H_{int} a term that takes into account interactions between the particles. Hence, H_0 represents the "easily" describable term while the terms $V(t) + H_{\text{int}}$ act as the perturbation. Our goal is then to develop a perturbation scheme, requiring us to work to in the interaction picture, in order to evaluate the expectation value of a certain observable O at times $t > t_0$, that is, to evaluate $\langle O \rangle(t) = \text{Tr}[\rho(t)O(t)]$ with $\rho(t)$ the density matrix in the Schrödinger picture obeying the Schrödinger equation

$$i\hbar \frac{d}{dt}\rho(t) = [H(t), \rho(t)] \tag{15}$$

Let us start by assuming that in the initial state of the system the density matrix at the reference time t_0 is given by

$$\rho(t_0) = \rho_0 \frac{1}{Z_0} e^{\beta_B(H_0 - \mu N)} \tag{16}$$

with μ the the chemical potential and $Z_0 = \text{Tr}\left[e^{-\beta_B(H_0-\mu N)}\right]$ the partition function for the equilibrium H_0. We can write $\rho(t)$ in terms of $\rho(t_0)$ in terms of the time-evolution operator as

$$\rho(t) = U(t, t_0)\, \rho(t_0)\, U(t_0, t) \;\text{ with } U(t_0, t) = e^{-i\hbar H(t - t_0)} \tag{17}$$

the time-evolution operator, which obeys the equations

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} U(t, t') &= H(t) U(t, t') \\ -i\hbar \frac{\partial}{\partial t'} U(t, t') &= U(t, t')\, H(t') \end{aligned} \tag{18}$$

and has with initial condition $U(t, t) = 1$. The evolution operator also satisfies $U(t, t_1)\, U(t_1, t') = U(t, t')$ and $U^{-1}(t, t') = U^{\dagger}(t, t') = U(t', t)$.

In order to do perturbation theory on $V(t) + H_{\text{int}}$ we will switch to the interaction picture. This is achieved by writing the time-evolution operator as

$$U(t, t') = U_0(t, t_0)\, S(t, t')\, U(t_0, t'), \;\text{ with } U_0(t, t') = e^{-i\hbar H_0 \left(t - t'\right)} \tag{19}$$

the time-evolution operator due to the unperturbed Hamiltonian and S an operator to determine, normally just called the S-matrix. It is easy to see that $S(t, t')$ obeys the equations

$$\begin{gathered} i\hbar \frac{\partial}{\partial t} S(t, t') = W(t) U(t, t') \;\text{ and }\; -i\hbar \frac{\partial}{\partial t'} S(t, t') = U(t, t')\, W(t') \\ \text{with } W(t) = U_0(t_0, t)\, [V(t) + H_{\text{int}}]\, U(t, t_0) \end{gathered} \tag{20}$$

the perturbation in the interaction picture. The S-matrix time evolution equations are also supplemented by the initial condition $S(t, t) = 1$. It's solution can be formally written as

$$S(t, t') = \begin{cases} T e^{-\frac{i}{\hbar}\int_{t'}^{t} dt_1 W(t_1)}, & t > t' \\ \bar{T} e^{\frac{i}{\hbar}\int_{t'}^{t} dt_1 W(t_1)}, & t < t' \end{cases} \tag{21}$$

with T the time-ordering operator and $\bar{T}$ the anti-time-ordering operator defined as

$$T c_\alpha(t) c_\beta^\dagger(t') = \begin{cases} c_\alpha(t) c_\beta^\dagger(t') & \text{for } t > t' \\ \zeta c_\beta^\dagger(t') c_\alpha(t) & \text{for } t < t' \end{cases} \tag{22}$$

$$\bar{T} c_\alpha(t) c_\beta^\dagger(t') = \begin{cases} \zeta c_\beta^\dagger(t') c_\alpha(t) & \text{for } t > t' \\ c_\alpha(t) c_\beta^\dagger(t') & \text{for } t < t' \end{cases} \tag{23}$$

with $\zeta = \pm 1$ representing either a commutator for bosonic operators or an anti-commutator for fermionic operators, respectively. If one of the two operators are neither bosonic nor fermionic, for example, they could be spin or angular momentum operators, there is no clear indication of the choice for ζ.

Finally, from these definitions we can write the expectation value of an operator in terms of the S-matrix, reading

$$\langle O \rangle(t) = \mathrm{Tr}[\rho(t) O(t)] = \mathrm{Tr}\left[\rho(t_0) S(t_0, t) O(t) S(t, t_0)\right] \equiv \langle S(t_0, t) O(t) S(t, t_0) \rangle_0 \tag{24}$$

since, in the interaction picture, $O(t) = U_0(t, t_0)\, O(t) U_0(t, t_0)$. See that, from this treatment, we were able to express the expectation value in terms of respect to the unperturbed "easy" density matrix ρ_0 instead of the total ρ. Moreover, expanding the S-operator in a Taylor series we obtain

$$\begin{aligned} \langle O \rangle(t) = \sum_{n,m} \frac{1}{n! m!} \left(\frac{i}{\hbar}\right)^n \left(-\frac{i}{\hbar}\right)^m \int_{t_0}^t dt_1 \ldots \int_{t_0}^t dt_n \int_{t_0}^t dt'_1 \ldots \int_{t_0}^t dt'_m \times \\ \times \left\langle \bar{T}\left[W(t_1) \ldots W(t_n)\right] O(t) T\left[W(t'_1) \ldots W(t'_n)\right] \right\rangle_0 \end{aligned} \tag{25}$$

effectively reducing the problem to the evaluation of a series of products of operators with respect to the the "easy" density matrix. To deal with such series of products of operators taken with respect to a density matrix of independent particles with next introduce the Wick's theorem.

B. Wick's theorem

Foremost, we mention that in this section we will not provide a full derivation of Wick's theorem but rather introduce it's result, accompanied with some intuition. For a full derivation see exercise.

Let us introduce the creation/annihilation operators notation $c_\alpha^\nu(t)$ with α a given state and t a given time step. For $\nu = +$ we have creation operators, $c_\alpha^+(t) = c_\alpha^\dagger(t)$, and for $\nu = -$ we have annihilation operator, $c_\alpha^-(t) = c_\alpha(t)$. Consider now the series of time-ordered fermionic operators taken with respect to a density matrix of independent particles

$$\left\langle c_{\alpha_1}^{\nu_1}(t_1) c_{\alpha_2}^{\nu_2}(t_2) \ldots c_{\alpha_n}^{\nu_N}(t_N) \right\rangle_0, \tag{26}$$

similar to what we arrived at at the end of the previous section. Wick's theorem states that for an even number of operators we have

$$\left\langle c_{\alpha_1}^{\nu_1}(t_1) c_{\alpha_2}^{\nu_2}(t_2) \ldots c_{\alpha_n}^{\nu_N}(t_N) \right\rangle_0 = \sum_{\text{pairings}} \zeta^P \left\langle c_{\alpha_{P(1)}}^{\nu_{P(1)}} c_{\alpha_{P(2)}}^{\nu_{P(2)}} \right\rangle_0 \ldots \left\langle c_{\alpha_{P(N-1)}}^{\nu_{P(N-1)}} c_{\alpha_{P(N)}}^{\nu_{P(N)}} \right\rangle_0, \tag{27}$$

where we sum over all possible combinations of the N operators with P the parity of the permutation that brings the operators in the order appearing in the left hand side into the order of the operators in each term of the right hand side, with $\zeta = +1$ for bosons and $\zeta = -1$ for fermions. Wick's theorem offers a significantly more practical method for evaluating the expectation value of a string of operators in systems composed of independent particles by effectively reducing the problem to one involving only

single-particle properties, encoded into the expectation values involving operator pairs, i.e $\left\langle c_{\alpha_i}^{\nu_i} c_{\alpha_j}^{\nu_j} \right\rangle_0$. Consequently, the expectation value of a longer string of operators can be written as a sum over products of such pairwise contractions. Since the particles involved are identical, all possible pairings of the operators must be considered. Furthermore, the nature of the particles, whether bosonic or fermionic, is essential in determining the sign associated with each term in the sum. In the case of bosonic operators, which commute, every term contributes positively. For fermionic operators, however, each term can carry either a positive or negative sign depending on the number of commutations required to bring the operators into the correct order for that particular contraction. As an additional note, see that in the absence of superconductivity, the only non-zero expectation values will be of the form $\left\langle c_{\alpha_i}^\dagger c_{\alpha_j} \right\rangle_0$ and $\left\langle c_{\alpha_i} c_{\alpha_j}^\dagger \right\rangle_0$.

Minimal example:

As a more concrete, practical, example, let us consider only fermionic operators and let us compute the string of expectation values $\left\langle c_\alpha c_\beta^\dagger c_\gamma^\dagger c_\delta \right\rangle_0$. According to Wick's theorem we have that

$$\begin{aligned}\left\langle c_\alpha c_\beta^\dagger c_\gamma^\dagger c_\delta \right\rangle_0 &= \left\langle \overbrace{c_\alpha c_\beta^\dagger}\, \overbrace{c_\gamma^\dagger c_\delta} \right\rangle + \left\langle \overbrace{c_\alpha c_\beta^\dagger c_\gamma^\dagger}\, c_\delta \right\rangle + \left\langle \overbrace{c_\alpha \overbrace{c_\beta^\dagger c_\gamma^\dagger} c_\delta} \right\rangle \\ &= \left\langle c_\alpha c_\beta^\dagger \right\rangle_0 \left\langle c_\gamma^\dagger c_\delta \right\rangle_0 + (-1) \left\langle c_\alpha c_\gamma^\dagger \right\rangle_0 \left\langle c_\beta^\dagger c_\delta \right\rangle_0 + (-1)^2 \left\langle c_\alpha c_\delta \right\rangle_0 \left\langle c_\beta^\dagger c_\gamma^\dagger \right\rangle_0\end{aligned}$$

See that in the first term, we get a plus sign because we did not alter the order of the operators, in the second term we get a minus sign because we made the anti-commutation $c_\beta^\dagger c_\gamma^\dagger \to (-1) c_\gamma^\dagger c_\beta^\dagger$ and finally, in the last term we get two negatives signs, amounting to a plus sign, due to the two commutations $c_\alpha c_\beta^\dagger c_\gamma^\dagger c_\delta \to (-1) c_\alpha c_\beta^\dagger c_\delta c_\gamma^\dagger \to (-1)^2 c_\alpha c_\delta c_\beta^\dagger c_\gamma^\dagger$. Another much simpler way to determine these signs in the case of fermions is by diagrammatic connecting with a line the two operators whom are being contracted, and then count the number of intersecting lines. If the number of intersections is even we get a plus sign, if the number is odd we get instead a negative sign.

C. Contour ordering

Now, armed with Wick's theorem, we know how to evaluate each term in the perturbative expansion of Eq.(25). However, it still have a double Taylor expansion, instead of a single one, which would be more desirable. To achieve such a single expansion, we start by noticing that in the products

$$\left\langle \bar{T} \left[W(t_1) \dots W(t_n) \right] O(t) T \left[W(t_1') \dots W(t_n') \right] \right\rangle_0 \tag{28}$$

from left to right, the operators first appear all time-ordered and then all anti-time-ordered. We can consider a directed double-time contour, $\mathcal{C}$, that initially goes forwards from t_0 to $t_{\max}$ (where $t_{\max}$ is greater than any t we are interested, for example, $t_{\max} \to \infty$) and then backwards from $t_{\max}$ to t_0. Such double-time contour can be parameterized by its arc-length s that goes from 0 to $2(t_{\max} - t_0)$ and that

$$t_{\mathcal{C}}(s) = \begin{cases} t_0 + s, & s \in [0, t_{\max} - t_0] \\ t_{\max} - (s - t_{\max} + t_0), & s \in [t_{\max} - t_0, 2(t_{\max} - t_0)] \end{cases} \tag{29}$$

Therefore we write $\mathcal{C} = \mathcal{C}^+ \cup \mathcal{C}^-$ with $C^{+/-}$ the forward/backwards contour. Moreover, we introducing the $\mathcal{C}$-contour-ordering operator as

$$T_{\mathcal{C}} \left[A(s_1) B(s_2) \right] = \begin{cases} A(s_1) B(s_2), & s_1 > s_2 \\ \zeta B(s_2) A(s_1), & s_1 < s_2 \end{cases}$$

noticing that the $\mathcal{C}^+$ $\mathcal{C}$-ordering corresponds to time-ordering while the $\mathcal{C}^-$ $\mathcal{C}$-ordering corresponds to anti-time-ordering. With these definitions we can write

$$\langle O\rangle(t) = \langle S\left(t_0,t\right) O(t) S\left(t,t_0\right)\rangle_0 = \langle T_{\mathcal{C}} S_{\mathcal{C}}\left(t_0,t_0\right) O(t)\rangle_0$$

$$\text{with } S_{\mathcal{C}}\left(t_0,t_0\right) = T_{\mathcal{C}} \exp\left[-\frac{i}{\hbar}\int_{\mathcal{C}} ds W(s)\right] \text{ and } W(s) \equiv W\left(t_{\mathcal{C}}(s)\right).$$

We point out that all that the operator $T_{\mathcal{C}}$ is doing is keeping the booking of which operators appear time-ordered or anti-time-ordered. If one is not interested in transient dynamics, we can take the limit $t_0 \to -\infty$, in which case, $\mathcal{C}$ is usually refereed to as the Schwinger-Keldysh contour.

To conclude, with this path trick, we obtain a single perturbative series expansion for $\langle O\rangle(t)$ reading

$$\langle O\rangle(t) = \sum_n \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_C ds_1 \ldots \int_C ds_n \left\langle T_C W\left(s_1\right)\ldots W\left(s_n\right) O(t)\right\rangle_0,$$

where the price we have paid is that the integrals $\int_{\mathcal{C}} ds_i$ is taken over the double-time contour $\mathcal{C}$. Maybe a figure for the path and to make more clear what we did where diagrammatically? And maybe a little paragraph with more intuition talk.

III. REAL TIME GREEN'S FUNCTIONS

A. Time-ordered, anti-time-ordered, greater and lesser GFs

Following the continuity of the previous section, when applying Wick's theorem to the result shown in Eq.(28) where the operators $O(t)$ evolves in the Heisenberg picture with $H(t)$, we obtain four different kinds of contractions. Specifically, these are either contractions between two operators that are time-ordered, contractions between two operators that are anti-time ordered or contractions between two operators that have a fixed order, $cc^\dagger$ or $c^\dagger c$. For this reason, we define and introduce what is called a Green's functions for each respective kind of contractions. These read as

$$\text{Time-ordered GF: } G^T_{\alpha\beta}(t,t') = -i\left\langle T_W c_\alpha(t) c^\dagger_\beta(t')\right\rangle \tag{30}$$

$$\text{Anti-time-ordered GF: } G^{\bar{T}}_{\alpha\beta}(t,t') = -i\left\langle \bar{T} c_\alpha(t) c^\dagger_\beta(t')\right\rangle \tag{31}$$

$$\text{Greater GF: } G^{>}_{\alpha\beta}(t,t') = -i\left\langle c_\alpha(t) c^\dagger_\beta(t')\right\rangle \tag{32}$$

$$\text{Lesser GF: } G^{<}_{\alpha\beta}(t,t') = -\zeta i\left\langle c^\dagger_\beta(t') c_\alpha(t)\right\rangle \tag{33}$$

The time-ordered and anti-time-ordered GFs are also commonly refer to as the causal and anti-causal GFs, respectively. Also, because two operators are involved in all these kind of GFs, there are sometimes collectively referred to as *two-time* GFs.

One can also define corresponding unperturbed Green's functions, where the operators evolve instead with the unperturbed H_0 and the expectation value is taken with respect to ρ_0. These unperturbed Green's function are usually denoted by a lower case g or with a index 0.

Notice that these four Green's functions are not linearly independent, but instead have the property

$$G^{>}_{\alpha\beta}(t,t') + G^{<}_{\alpha\beta}(t,t') = G^{T}_{\alpha\beta}(t,t') + G^{\bar{T}}_{\alpha\beta}(t,t')$$

1. Contour-ordered GFs

Moreover, motivated by the $\mathcal{C}$-contour-ordered treatment done above, it is also common to analogously define a $\mathcal{C}$-contour-ordered Green's function as

$$G^{\mathcal{C}}_{\alpha\beta}(s,s') = -i\left\langle T_{\mathcal{C}} c_\alpha(s) c^\dagger_\beta(s')\right\rangle$$

where the operators $O(s)$ evolve along the contour following the Heisenberg equation in the $\mathcal{C}$ contour.

Depending on whether the arguments of the contour-ordered GF lie in the $\mathcal{C}^+$ or $\mathcal{C}^+$ contour, these deduces to different real-time Green's functions, namely

$$\begin{aligned}
G^{\mathcal{C}}_{\alpha\beta}(t_+,t'_+) &= -i\left\langle T_{\mathcal{C}} c_\alpha(t_+) c^\dagger_\beta(t'_+)\right\rangle = -i\left\langle T c_\alpha(t) c^\dagger_\beta(t')\right\rangle = G^{T}_{\alpha\beta}(t,t') \\
G^{\mathcal{C}}_{\alpha\beta}(t_+,t'_-) &= -i\left\langle T_{\mathcal{C}} c_\alpha(t_+) c^\dagger_\beta(t'_-)\right\rangle = -\zeta i\left\langle c^\dagger_\beta(t'_-) c_\alpha(t_+)\right\rangle = G^{<}_{\alpha\beta}(t,t') \\
G^{\mathcal{C}}_{\alpha\beta}(t_-,t'_+) &= -i\left\langle T_{\mathcal{C}} c_\alpha(t_-) c^\dagger_\beta(t'_+)\right\rangle = -i\left\langle c_\alpha(t_-) c^\dagger_\beta(t'_+)\right\rangle = G^{>}_{\alpha\beta}(t,t') \\
G^{\mathcal{C}}_{\alpha\beta}(t_-,t'_-) &= -i\left\langle T_{\mathcal{C}} c_\alpha(t_-) c^\dagger_\beta(t'_-)\right\rangle = -i\left\langle \bar{T} c_\alpha(t) c^\dagger_\beta(t')\right\rangle = G^{\bar{T}}_{\alpha\beta}(t,t')
\end{aligned}$$

with $t^\pm$ referring to a time variable in the $\mathcal{C}^\pm$ contour. This relation follow directly from the fact that when both variables lie in $\mathcal{C}^+$ it reduces to time-ordering, when both variables lie in $\mathcal{C}^-$ it reduces to anti-time-ordering and when one variable lies in $\mathcal{C}^+$ and the other in $\mathcal{C}^-$, contour-ordering always puts the operator in $\mathcal{C}^-$ on the left. Is the greater and lesser GF are just the analytically continued GFs $G(\tilde{\omega} = \omega + i\eta)$ and $G(\tilde{\omega} = \omega - i\eta)$?

B. Retarded and advanced GFs

Besides all these GFs definitions there is two more, known as the retarded and advanced GFs. There are defined in terms of the Heaviside theta function $\Theta(t-t')$, reading

$$\text{Retarded GF: } G^R_{\alpha\beta}(t,t') = -i\Theta(t-t')\left\langle \left[c_\alpha(t), c^\dagger_\beta(t')\right]_\zeta \right\rangle \tag{34}$$

$$\text{Advanced GF: } G^A_{\alpha\beta}(t,t') = i\Theta(t'-t)\left\langle \left[c_\alpha(t), c^\dagger_\beta(t')\right]_\zeta \right\rangle \tag{35}$$

Understand that these definitions were not arbitrary chosen but were hinted by the time-ordered GF definition. Expressed in terms of the same Heaviside theta function $\Theta(t-t')$ it reads

$$G^T_{\alpha\beta}(t,t') = \Theta(t-t') c_\alpha(t) c^\dagger_\beta(t') + \zeta\Theta(t-t') c^\dagger_\beta(t') c_\alpha(t)$$

where the notation $\left[c_\alpha(t), c^\dagger_\beta(t')\right]_\zeta$ denotes both the bosonic commutator for $\zeta = +1$ and the fermionic anti-commutator for $\zeta = -1$. See that the retarded GF is nonzero only when $t > t'$, whereas the reverse is true for the advanced GF, leading to implications regarding causality. Moreover, see also that that none of the four causal, anti-causal, retarded and advanced GFs are defined at $t = t'$ because of the Heaviside theta function discontinuity. Furthermore, one of the simple properties of all these GFs is that they depend on the time labels t and t' only through their difference $t - t'$. (see exercise ?).

The retarded and advanced Green's functions are related to the previous ones as

$$\begin{aligned}
G^R_{\alpha\beta}(t,t') =& G^T_{\alpha\beta}(t,t') - G^<_{\alpha\beta}(t,t') = G^>_{\alpha\beta}(t,t') - G^{\bar{T}}_{\alpha\beta}(t,t') \\
G^A_{\alpha\beta}(t,t') =& G^T_{\alpha\beta}(t,t') - G^>_{\alpha\beta}(t,t') = G^<_{\alpha\beta}(t,t') - G^{\bar{T}}_{\alpha\beta}(t,t')
\end{aligned}$$

We also have the two additional relations

$$G^R_{\alpha\beta}(t,t') - G^A_{\alpha\beta}(t,t') = G^>_{\alpha\beta}(t,t') - G^<_{\alpha\beta}(t,t')$$
$$G^R_{\alpha\beta}(t,t') + G^A_{\alpha\beta}(t,t') = G^T_{\alpha\beta}(t,t') - G^{\bar{T}}_{\alpha\beta}(t,t')$$

Explain from these relations why we focus more on the retard, advanced and causal but specifically on the retard.

C. Equations of motion

Let us study now briefly discuss how the GFs evolve in time by differentiate them with respect to t. It may easily be verified that exactly the same final result will hold for all the four retarded, advanced, causal and anti-causal GFs, even though some of the intermediate steps are different. We can then write quite generally (dropping the R, A, C and $\bar{C}$ subscripts) for a generic operator A and B that

$$\frac{d}{dt}G\left(c_\alpha(t), c^\dagger_\beta(t')\right) = -\delta(t-t')\left\langle\left[c_\alpha(t), c^\dagger_\beta(t')\right]_\zeta\right\rangle + iG\left([H, c_\alpha(t)]\,; c^\dagger_\beta(t')\right) \tag{36}$$

where, given the different nature of the last term, we introduced the shorthand notations $G\left(A(t); B(t')\right)$ such that $G_{\alpha\beta}\left(t-t'\right) \equiv G\left(c_\alpha(t), c^\dagger_\beta(t')\right)$.

D. Spectral representation

Consider now a generic one-body operator defined as

$$J(t,t') = \sum_{\alpha\beta} J_{\alpha\beta}(t,t') c^\dagger_\alpha(t) c_\beta(t'). \tag{37}$$

with $J_{\alpha\beta}$ the spectral function, also called spectral intensity. As we will understand latter, for equilibrium system it encodes the information about the spectrum of the system since it provides us with a measure of the strength associated with each frequency in the Fourier spectrum. We introduce its definition here, reading

$$J_{\alpha\beta}(t,t') = \frac{1}{\hbar}\left\langle\left[c_\alpha(t), c^\dagger_\beta(t')\right]_\zeta\right\rangle = i\left(G^R_{\alpha\beta}(t,t') - G^A_{\alpha\beta}(t,t')\right)$$

The expectation value of the one-particle operator, this is, it's equilibrium thermal average at a given time t can be written in term of the causal Green function as

$$\langle J\rangle = -i\sum_{\alpha\beta} J_{\alpha\beta} G^T_{\beta\alpha}(t,t^+)$$

where the time stamp t' is taken to be at $t^+ = t+\eta$ with $\eta \to 0^+$. This t^+ time argument allows us, for example, to usefully define $\langle\rho(\mathbf{r},t)\rangle = -iG^T(\mathbf{r},t,\mathbf{r},t^+)$ with $\rho(\mathbf{r},t) = c^\dagger(\mathbf{r},t)c(\mathbf{r},t)$ the particle density.

Take now the inverse Fourier transform of a Green's function, $G_{\alpha\beta}(\omega) = \frac{1}{2\pi}\int dt G_{\alpha\beta}(t) e^{i\omega t}$, and the Fourier transform of the spectral function $J_{\alpha\beta}(t,t') = \int d\omega J_{\alpha\beta}(\omega) e^{-i\omega(t-t')}$. Making use of the Heaviside theta step-function and Dirac delta function integral representation (see exercise.VI.x), one obtains the relationship

$$G^T_{\alpha\beta}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega' J_{\alpha\beta}(\omega')\left\{\frac{e^{\beta_B\omega'}}{\omega-\omega'+i\eta} - \frac{\zeta}{\omega-\omega'-i\eta}\right\} \tag{38}$$

See that if one applies the same treatment instead to the retarded Green's function the denominations would both have $+i\eta$ which would lead to the canceling of the contribution of the number of states n_α. This is because...

Free electron gas example

Consider a single-particle non-interacting Hamiltonian given by $H_0 = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha$ with ε_α the energy of the α-defined state. Also, $\omega_\alpha = \varepsilon_\alpha/\hbar$ its frequency with $\hbar = 1$. From the Heisenberg equation of motion we have that $i\hbar\dot{c}_\alpha = [c_\alpha, H_0] = \varepsilon_\alpha c_\alpha$ and thus $c_\alpha(t) = e^{-i\omega_\alpha t}c_\alpha(0)$. Following by direct substitution the causal Green's function in real-time space reads

$$G^T_{\alpha\beta}(t,t') = e^{-i\omega_\alpha(t-t')}\delta_{\alpha\beta}\left[-i\Theta(t-t')(1-n_\alpha) + i\Theta(t'-t)n_\alpha\right]. \tag{39}$$

where the same-time correlation function $\left\langle c_\alpha^\dagger c_\alpha \right\rangle$ is just the number of states dictated by the Fermi-Dirac $n_\alpha = 1/\exp\left(e^{\beta_B(\varepsilon_\alpha-\mu)}+1\right)$ with μ the chemical potential and β_B the Boltzman temperature. By performing it's Fourier transform whilst ensuring that the exponentials converge at $t = \pm\infty$ by inserting the factors $e^{\mp\eta t}$, the causal Green's function in frequency space will read

$$G^T_{\alpha\beta}(\omega) = \delta_{\alpha\beta}\frac{1-n_\alpha}{\omega-\omega_\alpha+i\eta} + \delta_{\alpha\beta}\frac{n_\alpha}{\omega-\omega_\alpha-i\eta} \tag{40}$$

with 1st term represents the contribution from the empty states while the 2nd from the filled states. For example, for a free electron gas system one would set $\alpha = (\mathbf{k},\sigma)$ with $\mathbf{k}$ momentum and σ spin. In this case, for the ground state at $T = 0$, the first term will vanishes $\varepsilon_k < \mu$ while the second term vanishes for $\varepsilon_k > \mu$.

E. Kramers–Kronig relations and fluctuation-dissipation theorem

Making use of the Cauchy principal value (see exercise IV)

$$\frac{1}{x \pm i\eta} = \mathcal{P}\left(\frac{1}{x}\right) \mp i\pi\delta(x)$$

, one can straightforward separate the real and and imaginary parts of the various GFs. Focusing on the retarded GF due to it's significance, one obtaining

$$\mathrm{Re}G^R_{\alpha\beta}(\omega) = \frac{1}{2\pi}\mathcal{P}\int_{-\infty}^{+\infty}d\omega'\int_{-\infty}^{+\infty}d\omega'\frac{J_{\alpha\beta}(\omega')\left(e^{\beta_B\omega'}-\zeta\right)}{\omega-\omega'} \tag{41}$$

$$\mathrm{Im}G^R_{\alpha\beta}(\omega) = -\frac{1}{2}\left(e^{\beta_B\omega}-\zeta\right)J_{\alpha\beta}(\omega) \tag{42}$$

In the same manner, one can show all three GFs have the same real part, i.e $\mathrm{Re}G^R_{\alpha\beta}(\omega) = \mathrm{Re}G^A_{\alpha\beta}(\omega) = \mathrm{Re}G^C_{\alpha\beta}(\omega)$, with their differences arise only from their imaginary parts, reading $\mathrm{Im}G^R_{\alpha\beta}(\omega) = -\mathrm{Im}G^A_{\alpha\beta}(\omega)$ and $\mathrm{Im}G^C_{\alpha\beta}(\omega)$ having $-\zeta \to +\zeta$.

Moreover, one may eliminate the $J_{\alpha\beta}(\omega)$ dependence within the integrand and re-express the right-hand side in terms of the imaginary parts of the corresponding GF, reading

$$\mathrm{Re}G^R_{\alpha\beta}(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}d\omega'\frac{\mathrm{Im}G^R_{\alpha\beta}(\omega)}{\omega-\omega'} \tag{43}$$

This results show that the real and imaginary parts of the GFs are intricately related through integral expressions, representing examples of the so-called Kramers–Kronig relations, which have a

more general validity for a class of complex functions that are analytic in either the upper or lower half of the complex plane. Also, it can be shown that the relationships obtained here are bidirectional in the sense that the imaginary part can be expressed as an integral over an expression that contains the real part. Hence, the Kramers–Kronig relations have allowed us to express the real (or imaginary) part of the GF in terms of its imaginary (or real) part.

Notably, see that the connection between the real and imaginary parts is particularly simple for the retarded and advanced GFs while for the causal GF one can check that there is an additional $(e^{\beta_B\omega'} - \zeta)/(e^{\beta_B\omega'} + \zeta)$ term. The significance of these may be viewed as a consequence in the frequency domain of the fact that the retarded and advanced GFs in the time domain are nonzero only when $t > t'$ or vice versa. They are related, therefore, to ideas of causality in these cases. We shall come back to this topic to explore some applications of the Kramers–Kronig relations in the context of linear response theory.

As a further result, see that one can rearrange the results obtained for the imaginary parts of the GFs so that they become expressions for the spectral intensity. This is a particularly important result because it provide a direct way of deducing the spectral function and consequentially the time correlation functions, once we have calculated any of the GFs. These results are known collectively as the fluctuation-dissipation theorem because in many physical applications the imaginary part of the GF may be related to the dissipative (or "frictional") effects in a system, while the spectral function contains information about the excitations (or "fluctuations") in a related property of the system.

A case of special interest is the high-temperature or classical regime where $\hbar\omega \ll k_B T$ for the relevant frequencies. In this case the fluctuation-dissipation theorem reduces to $J_{\alpha\beta}(\omega) = -2/(\beta_B\omega)\mathrm{Im}G^R_{\alpha\beta}(\omega)$.

1. *Local density of states*

From the fluctuation-dissipation theorem, and following from the (non-interacting) free electron gas example, the density of states (DoS) follows as

$$\mathrm{DoS} = -\sum_\alpha \frac{1}{\pi}\mathrm{Im}G^R_{\alpha\alpha}(\omega) = -\sum_\alpha \frac{1}{\pi}\mathrm{Im}\left(\frac{1}{\omega - \omega_\alpha + i\eta}\right) = \sum_\alpha \delta(\omega - \omega_\alpha). \tag{44}$$

If the α state is not steady but instead decays over some lifetime τ due to interaction then the retarded GFs becomes instead

$$G^R_{\alpha\alpha}(t) = -i\Theta(t)e^{-i\omega_\alpha t}e^{-t/\tau} = \frac{1}{\omega - \omega_\alpha + i\Gamma} \tag{45}$$

with $\Gamma = 1/\tau$ the decay rate. The spectral function becomes a broadened delta function of width Γ, dubbed a Lorentzian distribution and being denoted as δ_Γ, reading

$$\mathrm{DoS} = -\sum_\alpha \frac{1}{\pi}\mathrm{Im}G^R_{\alpha\alpha}(\omega) = -\sum_\alpha \frac{1}{\pi}\frac{\Gamma}{\omega - \omega_\alpha + \Gamma^2} \equiv \sum_\alpha \delta_\Gamma(\omega - \omega_\alpha).$$

I have the two Fourier transforms choices mixed. When revising I will make sure the πs are correct. Also, there are random $\hbar$ floating around.

IV. IMAGINARY TIME GREEN'S FUNCTIONS

The typical situation in interacting many-body systems is that there may be no systematic or rigorous procedures for calculating the real-time GFs, except for special cases. Nevertheless, there are various approximation methods that have been developed for the real-time GFs, and these will be covered in

the next few chapters of this book. By contrast, however, perturbation methods (usually expressed in terms of a diagrammatic representation) are applicable for another type of GF that is defined with imaginary-time labels.

The so-called imaginary-time or Matsubara GFs is formally defined as

$$G^M_{\alpha\beta}(\tau-\tau') = -\left\langle T c_\alpha(\tau) c^\dagger_\beta(\tau')\right\rangle \tag{46}$$

with τ denoting the imaginary time, distinct from the real-time t. These time labels are, however, still real values. In this formalism the time-dependence of the operators becomes, for example, $c^\dagger_\alpha(\tau) = e^{H\tau} c^\dagger_\alpha e^{-H\tau}$, with the difference being that, before, the exponents were pure imaginary, whereas now they are real. It is in this sense that τ, although being real parameters, play a role analogous to that for an "imaginary" time. We note here that care must be taken in forming the Hermitian conjugates of the τ-dependent operators. For example, it can easily be checked that $c^\dagger_\alpha(\tau) \neq [c_\alpha(\tau)]^\dagger$. In fact the Hermitian conjugate of $c^\dagger_\alpha(\tau)$ is $c^\dagger_\alpha(-\tau)$. Moreover, by analogy with the result found for the GFs in the real-time formalism, the imaginary-time GFs depend only on the difference $\tau - \tau'$ and this one only needs to consider the function $G^M_{\alpha\beta}(\tau)$ with τ' set to zero.

A. Discrete Matsubara frequencies

An important property of the imaginary-time GF is that is always periodic with a period equal to 2β, following from

$$G^M_{\alpha\beta}(\tau) = \zeta G^M_{\alpha\beta}(\tau+\beta_B) = G^M_{\alpha\beta}(\tau+2\beta_B) \tag{47}$$

Consequently, without loss of generality we are free to choose τ to satisfy $-\beta < \tau < \beta$. Also, because of this periodicity, it follows that we may expand the GF as a Fourier series in this chosen interval, reading

$$G^M_{\alpha\beta}(\tau) = \frac{1}{\beta_B}\sum_{m=-\infty}^{\infty} e^{i\omega_m\tau} G^M_{\alpha\beta}(i\omega_m) \text{ with } m\in\mathbb{Z} \tag{48}$$

and with the overall $1/\beta_B$ factor appearing only for later convenience. See that the frequencies (often called Matsubara frequencies) form a discrete set, rather than a continuous one, which is why we have a summation rather than an integration. Note, however, that in the zero-temperature limit (when $\beta_B \to \infty$) the interval between adjacent frequencies, given by $2\pi/\beta_B$, will become infinitely small to zero and thus the frequency spectrum can only be considered discreet as long as $T \neq 0$. Furthermore, see that they take different values for bosons and for fermions, being

$$\omega_m = \begin{cases} (2m+1)\,\pi/\beta & \text{for fermions } (\zeta=-1) \\ 2m\pi/\beta & \text{for bosons } (\zeta=+1) \end{cases} \tag{49}$$

See that the frequencies are always nonzero for fermions but can be zero for bosons when $m = 0$.

B. The Lehmann representation

Let us now consider only times $\tau > 0$ (still with τ' set to zero) such that, for two given operators A and B, the Matsubara GF $G^M(\tau) \equiv G^M(A;B|\tau)$ can be decomposed as (see exercise IV)

$$G^M(\tau) = -\langle A(\tau)B(0)\rangle = -\frac{1}{Q}\sum_{\alpha\beta} e^{-\beta_B\varepsilon_\alpha} e^{\tau(\varepsilon_\alpha-\varepsilon_\beta)} \langle\alpha|A|\beta\rangle\langle\beta|B|\alpha\rangle \tag{50}$$

where we made use of the completeness property of the states of the system, i.e $\sum_\alpha |\alpha\rangle \langle\alpha| = 1$. The inverse Fourier transform in frequency space will then read (see exercise IV)

$$G^M(i\omega_m) = \int_0^\beta d\tau e^{i\omega_m \tau} G^M(\tau) = \frac{1}{Q}\sum_{\alpha\beta} \frac{e^{-\beta_B \varepsilon_\alpha} - \zeta e^{-\beta_B \varepsilon_\beta}}{i\omega_m + \varepsilon_\alpha - \varepsilon_\beta} \langle\alpha| A |\beta\rangle \langle\beta| B |\alpha\rangle$$

where we made use of the fact that $\exp(i\omega_m \beta_B) = \zeta$ for the boson and fermion Matsubara frequencies. This is representation of the Matsubara GF is known as the Lehmann representation.

Following the same Lehmann representation treatment for the real-time counterpart one finds that by one can simply make the replacement $i\omega_m \to \omega + i\eta$ (besides an overall factor of $1/2\pi$ due to the conventions adopted for the respective Fourier transforms), meaning that, if one has already calculated the imaginary-time GF, one may directly obtain the corresponding retarded GF by said replacement.

V. DIAGRAMMATIC PERTURBATION METHODS

Instead of proceeding algebraically, which soon becomes tedious in terms of applying Wick's theorem and dealing with the preceding integrations over the τ labels, it is convenient to relate the GF formalism to a diagrammatic representation that makes it easier to keep track of all the terms when applying Wick's theorem. The diagrams are often referred to as Feynman diagrams following the pioneering work by Richard Feynman, who introduced a diagram representation in term of lines, representing a GF or "propagator" evolving in real time and interaction vertices. In the formalism to be presented here we shall, in fact, be using the imaginary-time GF, so there is no useful notion in the same sense of forward and backward propagation in time.

We begin by taking a concrete interaction term example and immediately representing it diagrammatic, after which we provide a detailed exposition of the underlying physical intuition and the formal rules governing the construction. Then, from this first diagram, we explain how to apply Wick's theorem from a diagrammatic standpoint.

A. Electron-electron interaction

Let us then start by considering the interacting term

$$H_{\text{int}}(\tau) = \frac{1}{2} V(\mathbf{q}) c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2} c_{\mathbf{k}_2+\mathbf{q}} c_{\mathbf{k}_2-\mathbf{q}}.$$

It's diagrammatic representation, known as the interaction vertex, is represented as

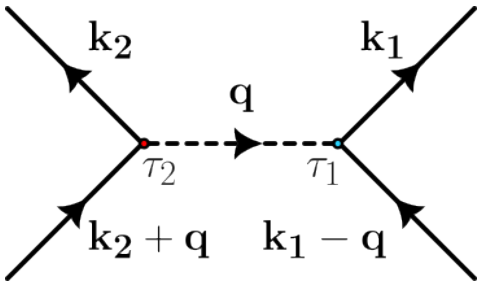


Figure 1. Electron-electron vertex diagram

Foremost, see that the inward-pointing propagators diagrammatically represent the annihilation operators, carrying the momentum labels $\mathbf{k}' + \mathbf{q}$ and $\mathbf{k} - \mathbf{q}$ of the penultimate and last terms respectively, which will eventually vanish for the sake of the interaction. Them, from that very same interaction, emerge the outward-pointing propagators diagrammatically representing the creation operators, carrying the momentum labels $\mathbf{k}'$ and $\mathbf{k}$ of the 2nd and 1st term respectively. Moreover, see that the interaction $V(\mathbf{q})$ is diagrammatically represented as the dashed line carrying the momentum label $\mathbf{q}$ and being labeled with the appropriate imaginary time τ. One way to conceptually interpret this diagram is to think of the propagators arrows as particles moving in that given direction, for example, electrons for full lines and a mediating particle for the dashed lines, be it a photon or a phonon or whatever, and the vertices as its collisions happening at a time τ.

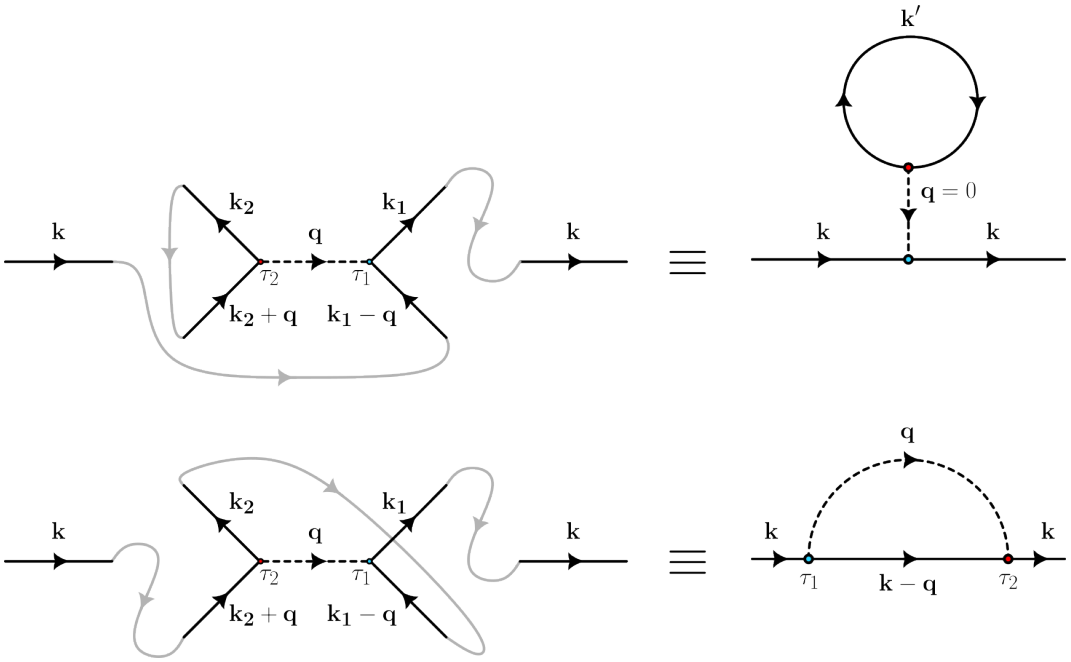


Figure 2. Electron-electron 1st order diagrams

Missing the 2nd order terms. In the exercise sheets I have how to make them but here I'm only interested in showing the final result.

This section is not even close to done. I will eventually get to it.

B. Dyson equation

We this section we introduce the concept of self energy, in particular, the concept of *proper* self-energy.

Analogously to how we handled the previous section, we immediately start from a concrete diagrammatic example, after which we provide a detailed exposition of the underlying physical and mathematical intuition. With no more further ado, let us consider the diagrams of some $G_{\mathbf{k}}(i\omega_m)$ shown in Fig.(**??**). Still need to incorporate a segue-way to the proper and improper self-energies figure.

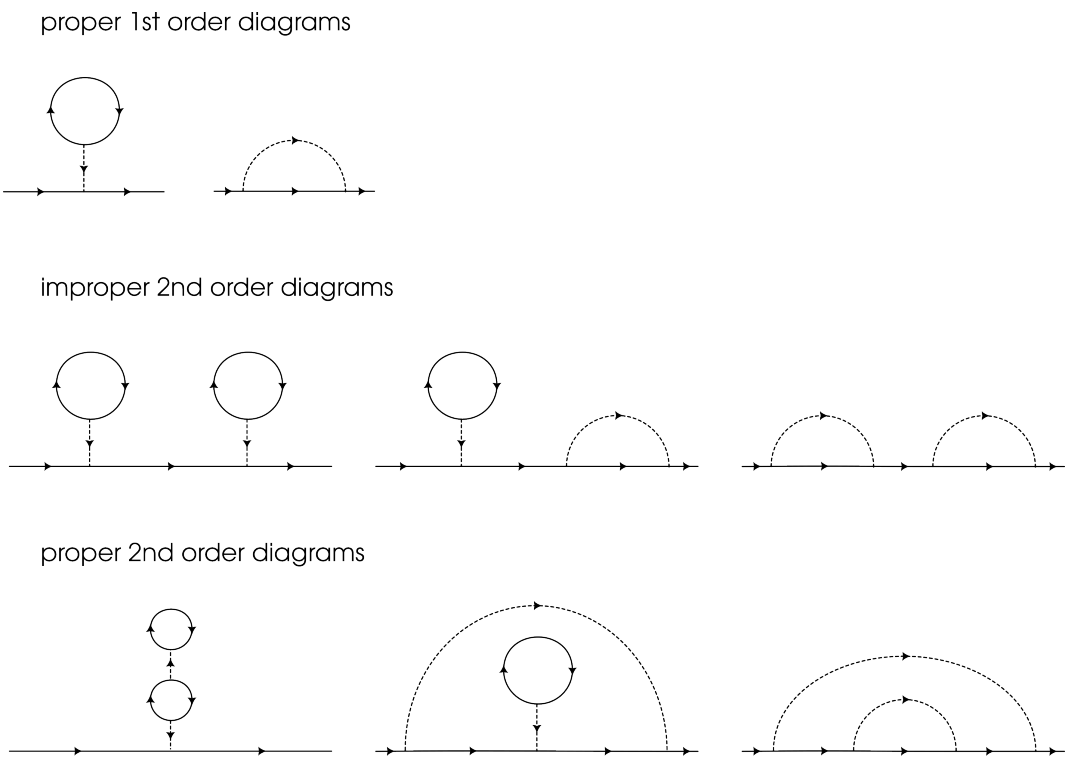


Figure 3. Proper versus improper diagrams

The summation of the series of diagrams represented in Fig.(4) can be encoded into the *proper* self-energy $\Sigma(\mathbf{k}, i\omega_m)$ and be represented as the series

$$\begin{aligned} G_{\mathbf{k}}(i\omega_m) &= G^0_{\mathbf{k}}(i\omega_m) \\ &+ G^0_{\mathbf{k}}(i\omega_m)\frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m)G^0_{\mathbf{k}}(i\omega_m) \\ &+ G^0_{\mathbf{k}}(i\omega_m)\frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m)G^0_{\mathbf{k}}(i\omega_m)\frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m)G^0_{\mathbf{k}}(i\omega_m) \\ &+ \ldots \end{aligned} \tag{51}$$

with $G^0_{\mathbf{k}}(i\omega_m)$ the Fourier-transformed imaginary-time GF for the unperturbed system, reading

$$G^0_{\mathbf{k}}(i\omega_m) = \frac{1}{i\omega_m - \varepsilon_{\mathbf{k}}} \tag{52}$$

Where this expression comes from is better explained in Cottam's, page 219. I will eventually incorporate it. Note that the self-energy Σ includes only proper interaction terms, while each nth order improper contribution being accounted for by nth successive term in the series.

It can be seen by a process of iteration with the last term on the right-hand side of the preceding expression that this is just the same as

$$G_{\mathbf{k}}(i\omega_m) = G^0_{\mathbf{k}}(i\omega_m) + G^0_{\mathbf{k}}(i\omega_m)\frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m)G_{\mathbf{k}}(i\omega_m) \tag{53}$$

The preceding result is known as Dyson's equation. It gives a connection between G and G^0 for any choice of the proper self-energy Σ. A separate calculation must be made for Σ using the diagrammatic rules.

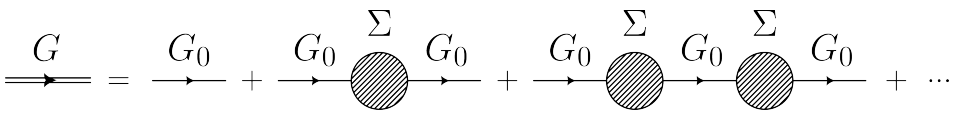


Figure 4. Dyson equation

Leaving aside the evaluation of Σ until later, we can easily rearrange Dyson's equation into an alternative form as

$$\left[G^0_{\mathbf{k}}(i\omega_m)\right]^{-1} = \left[G_{\mathbf{k}}(i\omega_m)\right]^{-1} + \frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m) \tag{54}$$

Moreover, substituting into the preceding equation the non-interacting GF $G^0_{\mathbf{k}}(i\omega_m)$ shown just above, the result for the interacting GF explicitly reads as

$$G_{\mathbf{k}}(i\omega_m) = \frac{1}{i\omega_m - \varepsilon_{\mathbf{k}} - \frac{1}{\beta}\Sigma(\mathbf{k}, i\omega_m)}. \tag{55}$$

In other words, the interacting GF is obtained from the non-interacting GF by making the formal replacement $\varepsilon_{\mathbf{k}} \to \varepsilon_{\mathbf{k}} + 1/\beta \times \Sigma(\mathbf{k}, i\omega_m)$

(56)

VI. GRASSMANN VARIABLES

A. Bosonic coherent states

B. Fermionic coherent state

Part II
Applications of Green's functions formalism

VII. EXACT METHODS OF GREEN'S FUNCTIONS FORMALISM

A. Non-interacting fermion gas

B. Light-matter interaction

1. Jaynes-Cummings two-level model

C. Dipole-exchange Ferromagnet

1. Heisenberg model

2. Ising model