A refresher in many-body theory

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1. QUANTUM MECHANICS FOR INTERACTING SYSTEMS IN CONDENSED MATTER

1.1 Introduction

The purpose of these notes is to point out a few key results in quantum mechanics, statistical physics and many-body theory that should be useful to understand the application of advanced numerical methods to condensed matter. The degree of sophistication necessary to understand these methods is very high. The important developments in the field have been achieved by people familiar with all the anlytical tricks of the trade.

These notes will not be very useful to learn the topics if you have never heard of them before. They should be seen as a summary of important concepts and methods to know in the context of this School.

1.2 Statistical Physics and Density matrix

1.2.1 Density matrix in ordinary quantum mechanics

Quantum mechanics tells us that the expectation value of an observable O in a *normalized* state $|\psi\rangle$ is given by $\langle\psi|\,O\,|\psi\rangle$. Expanding over complete sets of states, we obtain

$$\langle\psi|\,O\,|\psi\rangle \quad = \quad \sum_{i,j} \langle\psi|\,i\rangle\,\langle i|\,O\,|j\rangle\,\langle j\,|\psi\rangle \tag{1.1}$$

$$= \quad \sum_{i,j} \langle j\,|\psi\rangle\,\langle\psi|\,i\rangle\,\langle i|\,O\,|j\rangle \tag{1.2}$$

$$= \quad \sum_{i,j} \langle j|\,\rho\,|i\rangle\,\langle i|\,O\,|j\rangle \tag{1.3}$$

$$= \quad \mathrm{Tr}\,[\rho O] \tag{1.4}$$

where the *Density Matrix* ρ is defined, as an operator, by

$$\rho \equiv |\psi\rangle\,\langle\psi|\,. \tag{1.5}$$

This is when we have a *pure* state. If the state is prepared in a statistical superposition, in other words, if we have a certain probability p_n that the state that is prepared is $|\psi_n\rangle$, then the expectation value of an observable will be given by the weighted sum of the results in each state, in other words, in the above

formula for the average we should use

$$\rho \equiv \sum_n p_n \left| \psi_n \right\rangle \left\langle \psi_n \right|. \tag{1.6}$$

This is the density matrix for a *mixed state*. Note that

$$\rho^2 = \sum_{n,m} p_n p_m \left| \psi_n \right\rangle \left\langle \psi_n \right| \psi_m \right\rangle \left\langle \psi_m \right|. \tag{1.7}$$

We have the property $\rho^2 = \rho$ only for a *pure* state.

When a system of interest is in contact with an environment, it is very useful to work with an effective density matrix obtained by taking the trace first over the degrees of freedom of the environment. This idea is common in particular in the field of quantum information. In this school, we will see that by considering part of a large system as the environment, we can greatly reduce the size of the Hilbert space that needs to be considered to diagonalize a Hamiltonian, especially in one dimension. The optimal way of doing this was found by Steve White and will be discussed in the context of the "Density Matrix Renormalization Group". Not so surprisingly, quantum information theory has helped to improve even further this approach. Uli Schollwöck will explain this.

1.2.2 Density Matrix in Statistical Physics

Statistical Physics tells us that conserved quantities play a special role. Indeed, at equilibrium, the density matrix cannot depend on time, so it depends only on conserved quantities. This means that generally, the density matrix is diagonal in the energy and number basis for example. All that is left to do is to specify p_n. The basic postulate of statistical physics is that in an isolated system, all mcroscopic states consistent with the value of the conserved quantities are equiprobable. This is the microcanonical ensemble where p_n is identical for all energy eigenstates $\left| \psi_n \right\rangle$. The other ensembles are derived in the usual way by considering the microcanonical system as including the system of interest and various reservoirs. In the canonical ensemble for example, $p_n = e^{-\beta E_n}/Z$ where Z is the partition function $\sum_n e^{-\beta E_n}$ and $\beta = (k_B T)^{-1}$.

Alternatively, the various ensembles are obtained by maximizing the entropy

$$S \equiv -k_B \mathrm{Tr} \left[\rho \ln \rho \right] \tag{1.8}$$

subject to constraints such as fixed average energy and normalization in the case of the canonical ensemble. Important properties of the entropy include extensivity and concavity. The entropy also plays a major role in quantum information.

1.2.3 Legendre transforms

Legendre transforms are encountered in mechanics when going from a Lagrangian to a Hamiltonian formulation. That transformation is extremely useful in statistical physics as well and it will be used for example by Gabi Kotliar at this School.

The important idea of statistical physics that we start with is that of potentials. If you know the entropy as a function of mechanical quantities, like energy volume

and number of particles for example, then you know all the thermodynamics. Indeed,

$$dE = TdS - pdV + \mu dN \tag{1.9}$$

$$dS = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dN \tag{1.10}$$

so you can obtain temperature T, pressure p and chemical potential μ simply by taking partial derivatives of the entropy. $(1/T, S)\,(p/T, V)\,(-\mu/T, N)$ are pairs of conjugate variables. Instead of using E, V, N as independent variables, given the concavity of the entropy and the uniqueness of the equilibrium state, you can write S as a function of any three other variables. Nevertheless, the purely mechanical variables E, V, N are the most natural ones for the entropy. The entropy plays the role of a thermodynamic potential. As a function of all microscopic variables not fixed by E, V, N, it is maximum at equilibrium.

Remark 1 *When there are broken symmetries, additional variables must be added. For example, for a ferromagnet with magnetization* **M** *in a magnetic field* **H**,

$$dE = TdS - pdV + \mu dN + \mathbf{M} \cdot d\mathbf{H} \tag{1.11}$$

There are other potentials. For example, if a system is in contact with a heat reservoir, the work that will be done at constant temperature will be modified by the presence of the reservoir. It is thus physically motivated to define for example the Helmholtz free energy

$$F = E - TS \tag{1.12}$$

$$T = \left(\frac{\partial E}{\partial S}\right)_{V,N} \tag{1.13}$$

In this case

$$dF = dE - SdT - TdS = -SdT - pdV + \mu dN. \tag{1.14}$$

The Helmholtz free energy F can be written in terms of any three thermodynamical variables, but T, V, N are the most natural ones. At fixed T, V, N it is the free energy that is a minimum instead of the energy because we have to take into account the reservoir. The change from S to T as a natural variable has been done through the pair of equations (1.12,1.13). This is the general structure of a Legendre transform. F and E are potentials, and the subtraction of the product of the conjugate variables $-\left(\frac{\partial E}{\partial S}\right)_{V,N} S$ does the trick of relating the two potentials

Remark 2 *Note that* $\left(\partial^2 E/\partial S^2\right) = \left(\partial T/\partial S\right) = 1/\left(\partial S/\partial T\right) = -1/\left(\partial^2 F/\partial T^2\right).$

1.2.4 Legendre transform from the statistical mechanics point of view

Note that since

$$-\frac{F}{T} = S - \frac{E}{T} \tag{1.15}$$

$$= S - \left(\frac{\partial S}{\partial E}\right)_{V,N} E \tag{1.16}$$

the quantity $-F/T$ can be seen as the Legendre transform of the microcanonical entropy. From the point of view of statistical mechanics, if we define $\Omega\left(E\right)$ as the

number of microstate n corresponding to a given energy, then $p_n = 1/\Omega(E)$ for every microstate and

$$
\begin{aligned}
S(E) &= -k_B \mathrm{Tr}\left[\rho \ln \rho\right] = -k_B \sum_n \frac{1}{\Omega(E)} \ln \frac{1}{\Omega(E)} & (1.17) \\
&= k_B \ln \Omega(E) & (1.18)
\end{aligned}
$$

So, from the point of view of statistical mechanics, the Legendre transform of the entropy is obtained from

$$
\begin{aligned}
-\frac{F}{T} &= k_B \ln Z = k_B \ln \sum_n e^{-\beta E_n} & (1.19) \\
&= k_B \ln \sum_E \Omega(E) e^{-\beta E} & (1.20) \\
&= k_B \ln \sum_E e^{\ln \Omega(E)} e^{-\beta E} & (1.21) \\
&= k_B \ln \sum_E e^{(S(E)-E/T)/k_B} & (1.22)
\end{aligned}
$$

Whereas the microcanonical entropy is a function of the energy of microstates, its Legendre transform is summed over energy and is a function of $1/T$, the coefficient of E in both the thermodynamical expression of the Legendre transform Eq.(1.17) and the statistical one Eq.(1.22).

We know that

$$
\begin{aligned}
\langle E \rangle &= -\frac{\partial \ln Z}{\partial \beta} \\
&= -\frac{\partial(-F/T)}{\partial(1/T)} & (1.23)
\end{aligned}
$$

which clarifies the connection between the statistical mechanics and thermodynamical definitions of Legendre transform. E in the case of thermodynamics is really the average energy from the statistical mechanical point of view. The last equation could have been written down directly from the statistical expression for $-F/T$.

1.3 Second quantization

1.3.1 Describing symmetrized or antisymmetrized states

States that describe identical particles must be either symmetrized, for bosons, or antisymmetrized, for fermions. To simplify the calculations, it is useful to use second quantization. As its name suggest, there is also an axiomatic way to introduce this method as a quantization of fields but here we will just introduce it as a calculational tool. The approach will be familiar already if you master ladder operators for the harmonic oscillator.

For definiteness, let us concentrate on fermions. This can be translated for bosons. Define the operator $\psi^\dagger(\mathbf{r})$ that creates a particle in a position eigenstate

$|\mathbf{r}\rangle$ and antisymmetrizes the resulting wave function. Define also the vacuum state $|0\rangle$ that is destroyed by the adjoint, namely $\psi(\mathbf{r})|0\rangle = 0$. In this language

$$\psi^\dagger(\mathbf{r})\,\psi^\dagger(\mathbf{r}')\,|0\rangle \quad = \quad \frac{1}{\sqrt{2}}\left(|\mathbf{r}\rangle\,|\mathbf{r}'\rangle - |\mathbf{r}'\rangle\,|\mathbf{r}\rangle\right) \tag{1.24}$$

$$\equiv \quad |\mathbf{r},\mathbf{r}'\rangle = -\,|\mathbf{r}',\mathbf{r}\rangle\,. \tag{1.25}$$

The state to the right is clearly normalized and antisymmetric. There are two copies of the one-particle Hilbert space. In one component of the wave function, the particle in the first copy is at $|\mathbf{r}\rangle$, in the other component the particle in the first copy is at $|\mathbf{r}'\rangle$. Clearly, that can become quite complicated. The two body-wave function $\langle \mathbf{r},\mathbf{r}'\,|\varphi\rangle$ is antisymmetric and in the case where there are only two one-particle states occupied it is a Slater determinant. Clearly, that becomes a mess. In terms of the creation-annihilation operators however, all we need to know is that by definition of these operators,

$$\psi^\dagger(\mathbf{r})\,\psi^\dagger(\mathbf{r}') + \psi^\dagger(\mathbf{r}')\,\psi^\dagger(\mathbf{r}) = 0. \tag{1.26}$$

We use the short-hand for anticommutation

$$\left\{\psi^\dagger(\mathbf{r})\,,\psi^\dagger(\mathbf{r}')\right\} = 0. \tag{1.27}$$

Taking the adjoint,

$$\{\psi(\mathbf{r})\,,\psi(\mathbf{r}')\} = 0. \tag{1.28}$$

The only thing missing is that

$$\left\{\psi(\mathbf{r})\,,\psi^\dagger(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}')\,. \tag{1.29}$$

That is a bit more complicated to show, but let us take it for granted. It is clear that if $\psi^\dagger(\mathbf{r})$ creates a particle, then $\psi(\mathbf{r})$ removes one (or destroys it). If the particles are at different positions, that can be done in any order. If $\mathbf{r} = \mathbf{r}'$, then it will matter if we create a particle before destroying it. If the creation occurs before the destruction, there will be one more particle to destroy. The Dirac delta function comes from normalization in the continuum. For discrete basis, we would have unity on the right.

1.3.2 Change of basis

A key formula for the "field" operators $\psi^\dagger(\mathbf{r})$ is the formula for basis change. Suppose that one has a new complete basis of one-particle states $|\alpha\rangle$. Then, we can change basis as follows:

$$|\mathbf{r}\rangle = \sum_\alpha |\alpha\rangle\,\langle\alpha|\,\mathbf{r}\rangle \tag{1.30}$$

Given the definition of creation operators, the creation operator $\psi^\dagger(\mathbf{r})$ for a particle in state $|\mathbf{r}\rangle$ is related to the creation operator $c_\alpha^\dagger$ for a particle in state $|\alpha\rangle$ by the analogous formula, namely

$$\psi^\dagger(\mathbf{r}) = \sum_\alpha c_\alpha^\dagger\,\langle\alpha|\,\mathbf{r}\rangle\,. \tag{1.31a}$$

This formula is quite useful.

1.3.3 Second quantized version of operators

One-body operators

If we know the matrix elements of an operator in the one-particle basis, the calculation of any observable can be reduced to some algebra with the creation-annihilation operators. In other words, not only states, but also operators corresponding to observables can be written using creation-annihilation operators. The expression for these operators is independent of the number of particles and formally analogous to the calculation of averages of operators in first quantized notation.

To be more specific, consider the operator for the density of particles at position $|\mathbf{r}\rangle$. It can be written as $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ as we prove now. Since $ABC - CAB = ABC + ACB - ACB - CAB$ the commutator ot this operator with $\psi^\dagger(\mathbf{r}')$ is,

$$\left[\psi^\dagger(\mathbf{r})\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right] = \psi^\dagger(\mathbf{r})\left\{\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\} - \left\{\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right\}\psi(\mathbf{r}) \quad (1.32)$$

$$= \delta(\mathbf{r}-\mathbf{r}')\psi^\dagger(\mathbf{r}) \quad (1.33)$$

We can now use the following little "theorem" on commutator of ladder operators:

Theorem 1 *If $[A,B] = \beta B$ and $|\alpha\rangle$ is an eigenstate of A with eigenvalue α, then $B|\alpha\rangle$ is an eigenstate of A with eigenvalue $\alpha+\beta$, as follows from $AB|\alpha\rangle - BA|\alpha\rangle = A(B|\alpha\rangle) - \alpha(B|\alpha\rangle) = \beta(B|\alpha\rangle)$.*

Since $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|0\rangle = 0$, the above implies that $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\left(\psi^\dagger(\mathbf{r}_1)|0\rangle\right) = \delta(\mathbf{r}-\mathbf{r}_1)\left(\psi^\dagger(\mathbf{r}_1)|0\rangle\right)$, and generally a state $\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\ldots|0\rangle$ is an eigenstate of $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ with eigenvalue $\delta(\mathbf{r}-\mathbf{r}_1) + \delta(\mathbf{r}-\mathbf{r}_2) + \ldots$ Clearly, the potential energy of identical electrons in a potential $V(\mathbf{r})$ can ve written

$$\int \psi^\dagger(\mathbf{r})V(\mathbf{r})\psi(\mathbf{r})d^3\mathbf{r}. \quad (1.34)$$

The same reasoning leads to the kinetic energy in the momentum basis, where it is diagonal

$$\int c^\dagger(\mathbf{k})\frac{\hbar^2\mathbf{k}^2}{2m}c(\mathbf{k})\frac{d^3\mathbf{k}}{(2\pi)^3}. \quad (1.35)$$

Returning to the position-space basis, we obtain

$$\int \psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right)\psi(\mathbf{r})d^3\mathbf{r}. \quad (1.36)$$

In other words, for any one-body operator, we can always obtain its second-quantized form in the one-particle basis $|\alpha\rangle$ where it is diagonal:

$$\sum_\alpha c_\alpha^\dagger \langle\alpha|O|\alpha\rangle c_\alpha = \sum_{\alpha,\beta} c_\alpha^\dagger \langle\alpha|O|\beta\rangle c_\beta. \quad (1.37)$$

If we change to an arbitrary basis

$$|\alpha\rangle = \sum_i |i\rangle\langle i|\alpha\rangle \quad (1.38)$$

the operator takes the form

$$\sum_{\alpha,\beta} c_\alpha^\dagger \langle\alpha|O|\beta\rangle c_\beta = \sum_{\alpha,i,j} c_\alpha^\dagger \langle\alpha|i\rangle\langle i|O|j\rangle\langle j|\alpha\rangle c_\alpha = \sum_{i,j} c_i^\dagger \langle i|O|j\rangle c_j. \quad (1.39)$$

Example 2 Let $\psi_\alpha^\dagger(\mathbf{r})$ be the creation operator for the position state $|\mathbf{r}\rangle$ with the spin $\alpha = \uparrow, \downarrow$. We know the matrix elements of all component of the spin operators in the basis where S_z is diagonal. Thus, from the last formula, we see that the three components of the spin operator are

$$\int \psi_\alpha^\dagger(\mathbf{r}) \left(\frac{\hbar}{2}\boldsymbol{\sigma}_{\alpha\beta}\right) \psi_\beta(\mathbf{r}) d^3\mathbf{r} \tag{1.40}$$

where, as usual, the Pauli matrices are given by $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

Two-body operators

Let us now consider a two-body operator such as the potential energy. It is diagonal in position-space. The Coulomb interaction

$$V_c(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \tag{1.41}$$

is an example. The second quantized Coulomb energy takes the form

$$\int V_c(\mathbf{r} - \mathbf{r}') \frac{1}{2} \left(\rho(\mathbf{r})\rho(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r})\right) d^3\mathbf{r}d^3\mathbf{r}' \tag{1.42}$$

where the $1/2$ comes from avoiding double-counting and $\delta(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r})$ is necessary not to count the interaction of an electron with itself. Including spin, the density operator is

$$\rho(\mathbf{r}) = \sum_\sigma \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}). \tag{1.43}$$

Substituting in the expression for the Coulomb interaction and using anti-commutation relations, we obtain

$$\frac{1}{2}\sum_{\sigma,\sigma'}\int V_c(\mathbf{r} - \mathbf{r}')\psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) d^3\mathbf{r}d^3\mathbf{r}'. \tag{1.44}$$

It is an interesting and not very long exercise to prove that formula (which happens to have the same form for bosons and fermions).

Let us change to some arbitrary basis. First notice that in terms of the potential energy operator $\hat{V}_c$

$$V_c(\mathbf{r} - \mathbf{r}') = \langle\mathbf{r}|\langle\mathbf{r}'|\hat{V}_c|\mathbf{r}\rangle|\mathbf{r}'\rangle. \tag{1.45}$$

Then, the change of basis

$$\psi_\sigma^\dagger(\mathbf{r}) = \sum_i c_{i\sigma}^\dagger \langle i|\mathbf{r}\rangle. \tag{1.46a}$$

leads to the following two-particle analog of the one-body operator Eq.(1.39) in an arbitrary basis

$$\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{ijkl}\langle i|\langle j|\hat{V}_c|k\rangle|l\rangle c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma'}c_{k\sigma}. \tag{1.47}$$

1.4 Hartree-Fock approximation

The Hartree-Fock approximation is the simplest approximation to the many-body problem. It is a mean-field theory of the full Hamiltonian, that we will call "The theory of everything". We will begin by writing it explicitly then proceed with two theorems that form the basis of this approximation.

1.4.1 The theory of everything

Gathering the results of the previous section, an electron gas interacting with a *static* lattice takes the form

$$
\begin{aligned}
H_{toe} &= \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V_{c,e-i}(\mathbf{r}) \right) \psi_{\sigma}(\mathbf{r}) \, d^3\mathbf{r} \\
&+ \frac{1}{2} \sum_{\sigma,\sigma'} \int V_c(\mathbf{r} - \mathbf{r}') \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \, d^3\mathbf{r} d^3\mathbf{r}' \quad (1.48)
\end{aligned}
$$

where $V_{c,e-i}(\mathbf{r})$ is the electron-ion Coulomb potential. The dynamics of the ions (phonons) can be added to this problem, but until the rest of these introductory notes, we shall take the lattice as static. We need the to allow the lattice to move to have the complete "theory of everything" we want to solve in this School. But the above is certainly a non-trivial start.

1.4.2 Variational theorem

The Ritz variational principle states that any normalized wave function satisfies

$$
\langle \psi | H | \psi \rangle \geq \langle \psi_0 | H | \psi_0 \rangle \tag{1.49}
$$

where $|\psi_0\rangle$ is the ground state wave function.

Proof. That follows easily by expanding $|\psi\rangle = \sum_i a_i |\psi_i\rangle$, where $H |\psi_i\rangle = E_i |\psi_i\rangle$, and using $E_0 \leq E_i$:

$$
\begin{aligned}
\langle \psi | H | \psi \rangle &= \sum_{i,j} a_j^* a_i \langle \psi_j | H | \psi_i \rangle = \sum_i |a_i|^2 E_i \\
&\geq E_0 \sum_i |a_i|^2 = \langle \psi_0 | H | \psi_0 \rangle \tag{1.50}
\end{aligned}
$$

∎

In the Hartree Fock approximation, we use the variational principle to look for the best one-body Green function for H_{toe}. In other words, we use our formula for a change of basis (there is no sum on repeated spin index here)

$$
\psi_{\sigma}^{\dagger}(\mathbf{r}) = \sum_i c_{i\sigma}^{\dagger} \langle i,\sigma | \mathbf{r},\sigma \rangle = \sum_i c_{i\sigma}^{\dagger} \phi_{i\sigma}^*(\mathbf{r}) \tag{1.51}
$$

$$
c_{i\sigma}^{\dagger} = \int d^3\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \langle \mathbf{r},\sigma | i,\sigma \rangle = \int d^3\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \phi_{i\sigma}(\mathbf{r}) \tag{1.52}
$$

and write our ground state wave function as

$$|\psi_{HF}\rangle = c_{1\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} \ldots c_{N/2\uparrow}^{\dagger} c_{N/2\downarrow}^{\dagger} |0\rangle . \tag{1.53}$$

Our variational parameters are the one-particle Green functions $\phi_{\sigma}^{*}(\mathbf{r})$. Note that the most general wave function would be a linear combination of wave functions of the type $|\psi_{HF}\rangle$, each with different one-particle states occupied.

1.4.3 Wick's theorem

To compute $\langle\psi_{HF}| H |\psi_{HF}\rangle$, we expand each of the creation-annihilation operators in the Hamiltonian Eq.(1.48) in the basis we are looking for, using the change of basis formula Eq.(1.51). Consider first the quadratic term and focus on the second quantized operators. We need to know

$$\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle \tag{1.54}$$

The key to compute such matrix elements is to simply use the anticommutation relations for the creation-annihilation operators and the fact that annihilation operators acting on the vacuum give zero. Let us do this slowly.

The anticommutation relations for the operators $c_{i\sigma}^{(\dagger)}$ are as follows:

$$\left\{c_{i\sigma}, c_{j\sigma'}^{\dagger}\right\} = \int d^{3}\mathbf{r} \int d^{3}\mathbf{r}' \phi_{i\sigma}^{*}(\mathbf{r}) \left\{\psi_{\sigma}(\mathbf{r}), \psi_{\sigma'}^{\dagger}(\mathbf{r}')\right\} \phi_{j\sigma'}(\mathbf{r}') \tag{1.55}$$

$$= \int d^{3}\mathbf{r} \phi_{i\sigma}^{*}(\mathbf{r}) \phi_{j\sigma'}(\mathbf{r}) = \delta_{i,j}\delta_{\sigma,\sigma'} \tag{1.56}$$

so

$$\langle 0| c_{i\uparrow} c_{i\uparrow}^{\dagger} |0\rangle = 1 - \langle 0| c_{i\uparrow}^{\dagger} c_{i\uparrow} |0\rangle = 1. \tag{1.57}$$

Generalizing this reasoning, we see that $\langle\psi_{HF}| \psi_{HF}\rangle = 1$. Now, $\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle$ will vanish if either i or j are not in the list of occupied states in $|\psi_{HF}\rangle$ since $c_{i\uparrow}^{\dagger}$ also annihilates the vacuum in the bra. If i and j are both in the list of occupied states, $\langle\psi_{HF}| c_{i\uparrow}^{\dagger} c_{j\uparrow} |\psi_{HF}\rangle = \delta_{i,j}$ since $c_{j\uparrow}$ will remove a particle in state j in $|\psi_{HF}\rangle$ while $c_{i\uparrow}^{\dagger}$ will remove a particle in state i in $\langle\psi_{HF}|$. If the list of particles is not the same in the bra and in the ket, the annihilation operators can be anticommuted directly to the vacuum and will destroy it. With this, we have that

$$\langle\psi_{HF}| \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^{2}\boldsymbol{\nabla}^{2}}{2m} + V_{c,e-i}(\mathbf{r})\right) \psi_{\sigma}(\mathbf{r}) d^{3}\mathbf{r} |\psi_{HF}\rangle \tag{1.58}$$

$$= \sum_{\sigma} \sum_{i=1}^{N/2} \int \phi_{i\sigma}^{*}(\mathbf{r}) \left(-\frac{\hbar^{2}\boldsymbol{\nabla}^{2}}{2m} + V_{c,e-i}(\mathbf{r})\right) \phi_{i\sigma}(\mathbf{r}) d^{3}\mathbf{r}. \tag{1.59}$$

To compute the expectation value of the interacting part of H_{toe} we need

$$\langle\psi_{HF}| c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{k\sigma'} c_{l\sigma} |\psi_{HF}\rangle . \tag{1.60}$$

Since $|\psi_{HF}\rangle$ is a direct product of wave functions for up and down spins, if the spins are different, we obtain

$$\langle\psi_{HF}| c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{k\sigma'} c_{l\sigma} |\psi_{HF}\rangle = \delta_{i,l}\delta_{j,k}. \tag{1.61}$$

If the spins are identical, something new happens. If the conditions $k = l$ or $i = j$ are satisfied, the expectation value vanishes because of the anticommutation

relations (Pauli principle). Consider k different from l. Since all we need is that the list of states created be the same as the list of states destroyed there are two possibilities

$$\langle \psi_{HF} | c_{i\sigma}^\dagger c_{j\sigma}^\dagger c_{k\sigma} c_{l\sigma} | \psi_{HF} \rangle = \delta_{i,l} \delta_{j,k} - \delta_{i,k} \delta_{j,l}. \tag{1.62}$$

The last contribution is known as the exchange contribution. The difference in sign comes from the anticommutation. All these results, including the cases $k = l$ or $i = j$ for same spin, can be summarized by

$$\langle \psi_{HF} | c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma} | \psi_{HF} \rangle = \delta_{i,l} \delta_{j,k} - \delta_{i,k} \delta_{j,l} \delta_{\sigma,\sigma'}. \tag{1.63}$$

The last result can be written as

$$\langle \psi_{HF} | c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma} | \psi_{HF} \rangle = \langle \psi_{HF} | c_{i\sigma}^\dagger c_{l\sigma} | \psi_{HF} \rangle \langle \psi_{HF} | c_{j\sigma'}^\dagger c_{k\sigma'} | \psi_{HF} \rangle \tag{1.64}$$
$$- \langle \psi_{HF} | c_{i\sigma}^\dagger c_{k\sigma'} | \psi_{HF} \rangle \langle \psi_{HF} | c_{j\sigma'}^\dagger c_{l\sigma} | \psi_{HF} \rangle. \tag{1.65}$$

A four point correlation function has been factored into a product of two-point correlation functions. For states such as $| \psi_{HF} \rangle$ that are single-particle states, creation operators are "contracted" in all possible ways with the destruction operators. This elegant form is a special case of Wick's theorem. It applies to expectation values of any number of creation and annihilation operators. The signs follow from anticommutation.

1.4.4   Minimization and Hartree-Fock equations

Using Wick's theorem Eq.(1.63) and proceeding with the Coulomb interaction between electrons as we did with the one-body part of the Hamiltonian in Eq.(1.59) we obtain

$$\langle \psi_{HF} | H_{toe} | \psi_{HF} \rangle = \sum_\sigma \sum_{i=1}^{N/2} \int \phi_{i\sigma}^* (\mathbf{r}) \left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V_{c,e-i} (\mathbf{r}) \right) \phi_{i\sigma} (\mathbf{r}) \, d^3\mathbf{r}$$

$$+ \sum_{\sigma,\sigma'} \sum_{i=1}^{N/2} \sum_{j=1}^{N/2} \frac{1}{2} \int V_c (\mathbf{r} - \mathbf{r}') \left[\phi_{i\sigma}^* (\mathbf{r}) \phi_{i\sigma} (\mathbf{r}) \phi_{j\sigma'}^* (\mathbf{r}') \phi_{j\sigma'} (\mathbf{r}') \right. \tag{1.66}$$

$$\left. - \delta_{\sigma,\sigma'} \phi_{i\sigma}^* (\mathbf{r}) \phi_{i\sigma} (\mathbf{r}') \phi_{j\sigma'}^* (\mathbf{r}') \phi_{j\sigma'} (\mathbf{r}) \right] d^3\mathbf{r} \, d^3\mathbf{r}'. \tag{1.67}$$

To find our variational parameters, namely the functions $\phi_{i\sigma} (\mathbf{r})$, we minimize the above, subject to the constraint that the wave functions must be orthonormalized. This means that we take partial derivatives with respect to all variables in the above expression. We satisfy the constraints

$$\int \phi_{i\sigma}^* (\mathbf{r}) \phi_{j\sigma'} (\mathbf{r}) \, d^3\mathbf{r} - \delta_{i,j} \delta_{\sigma,\sigma'} = 0 \tag{1.68}$$

using Lagrange multipliers. We have to think of $\phi_{i\sigma}^* (\mathbf{r})$ and $\phi_{i\sigma} (\mathbf{r})$ as independents variable defined at each different position $\mathbf{r}$ and for each index i, σ. To take the partial derivatives carefully, one should discretize space and take the limit but the final result is pretty obvious. All we need to know is that what replaces the partial derivative in the continuum version is the functional derivative

$$\frac{\delta \phi_{i\sigma} (\mathbf{r})}{\delta \phi_{j\sigma'} (\mathbf{r}')} = \delta (\mathbf{r} - \mathbf{r}') \delta_{i,j} \delta_{\sigma,\sigma'} \tag{1.69}$$

$$\frac{\delta \phi_{i\sigma}^* (\mathbf{r})}{\delta \phi_{j\sigma'} (\mathbf{r}')} = 0. \tag{1.70}$$

The result of the minimization with respect of $\phi_{i\sigma}^*(\mathbf{r})$ is straightforward. One obtains

$$\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V_{c,e-i}(\mathbf{r})\right)\phi_{i\sigma}(\mathbf{r}) + V_H(\mathbf{r})\phi_{i\sigma}(\mathbf{r}) - \int d^3\mathbf{r}' V_{ex}(\mathbf{r},\mathbf{r}')\phi_{i\sigma}(\mathbf{r}')$$

$$= \sum_{i=1}^{N/2}\gamma_{ij}\phi_{j\sigma}(\mathbf{r}) \tag{1.71}$$

$$V_H(\mathbf{r}) = \int d^3\mathbf{r}' V_c(\mathbf{r}-\mathbf{r}')\sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r}')\right|^2 \tag{1.72}$$

$$V_{ex}(\mathbf{r},\mathbf{r}') = V_c(\mathbf{r}-\mathbf{r}')\sum_{j=1}^{N/2}\phi_{j\sigma}^*(\mathbf{r}')\phi_{j\sigma}(\mathbf{r}). \tag{1.73}$$

The matrix γ_{ij} is a real symmetric matrix of Lagrange multipliers. Diagonalizing γ_{ij} and writing the eigenvalues ε_i, the above equation looks like a Schrödinger equation. The Hartree contribution $V_H(\mathbf{r})$ has the physical interpretation that each electron interacts with the average density of the other electrons

$$n(\mathbf{r}) = \sum_{\sigma'}\sum_{j=1}^{N/2}\left|\phi_{j\sigma'}(\mathbf{r})\right|^2. \tag{1.74}$$

The exchange contribution $V_{ex}(\mathbf{r},\mathbf{r}')$ has no classical analog. It comes from the anticommutation of indistinguishible particles. The ε_i can be interpreted as single-particle excitation energies only if removing a particle does not modify too much the effective potentials.

1.5   Model Hamiltonians

Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. Nevertheless, it does not diagonalize the Hamiltonian. If the problem has been solved for a translationally invariant lattice, the one-particle states will be Bloch states indexed by crystal momentum $\mathbf{k}$ and band index n. If we expand the creation-annihilation operators in that basis using the general formulas for one-particle Eq.(1.39) and two-particle Eq.(1.47) parts of the Hamiltonian, clearly it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

Model Hamiltonians can now explicitly be constructed using cold atoms in optical traps. A laser interference pattern can be used to create an optical lattice potential using the AC Stark effect. One can control tunneling between potential minima as well as the interation of atoms between them.

1.5.1 The Hubbard model

Restricting ourselves to a single band and expanding in the Wannier basis associated with the Bloch states, the Hamiltonian takes the form

$$H = \sum_{\sigma} \sum_{i,j} c_{i\sigma}^{\dagger} \langle i| \hat{K} |j\rangle c_{j\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{ijkl} \langle i| \langle j| \hat{V}_c |k\rangle |l\rangle c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{l\sigma'} c_{k\sigma}. \quad (1.75)$$

where $\hat{K}$ contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. The operator $c_{i\sigma}^{(\dagger)}$ annihilate (create) a particle in a Wannier state centered at lattice site i and with spin σ. The one-body part by itself is essentially the DFT band structure. In 1964, Hubbard, Kanamori and Gutzwiller did the most dramatic of approximations, hoping to have a model simple enough to solve. They assumed that $\langle i| \langle j| \hat{V}_c |k\rangle |l\rangle$ would be much larger than all other interaction matrix elements when all lattice sites are equal. Defining $t_{ij} \equiv \langle i| \hat{K} |j\rangle$ and $U \equiv \langle i| \langle i| \hat{V}_c |i\rangle |i\rangle$, and using $c_{i\sigma} c_{i\sigma} = 0$ they were left with

$$\begin{aligned}
H &= \sum_{\sigma} \sum_{i,j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{i} U c_{i\sigma}^{\dagger} c_{i\sigma'}^{\dagger} c_{i\sigma'} c_{i\sigma} \\
&= \sum_{\sigma} \sum_{i,j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow} \quad (1.76) \\
&= \sum_{\sigma} \sum_{i,j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow}. \quad (1.77)
\end{aligned}$$

Most of the time, one considers hopping only to nearest neighbors. The model can be solved exactly only in one dimension using the Bethe ansatz, and in infinite dimension. The latter solution is the basis for Dynamical Mean Field Theory (DMFT) that will be discussed at this School. Despite that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable. The laser intensity of the trapping potential and the magnetic field are the control parameters. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of cold atoms, one can find conditions where the Hubbard model description is very accurate. By the way, interesting physics occurs only in the nano Kelvin range. Discussing how such low temperatures are achieved would distract us to much.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a Mott insulator. The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe high-temperature superconductivity, depending on lattice and range of interaction parameters.

1.5.2 Heisenberg and t-J model

Suppose we are in the limit where U is much larger than the bandwidth. One expects that in low energy eigenstates, single-particle Wannier states will be either

empty or occupied by a spin up or a spin down electron and that double occupation will be small. If we could write an effective Hamiltonian valid at low energy, that means that we would reduce the size of the Hilbert space from roughly 4^N to 3^N for an N site lattice. This is possible. The effective Hamiltonian that one obtains in this case is the $t-J$ model, which becomes the Heisenberg model at half-filling.

To obtain this model, one can use canonical transformations or equivalently degenerate perturbation theory. Although both approches are equivalent, the one that is most systematic is the canonical transformation approach. Nevertheless, we will see a simplified version of the degenerate perturbation theory approach since it is sufficient for our purpose and simpler to use.

We start from the point of view that the unperturbed part of the Hamiltonian is the potential energy. If there is no hopping, the ground state has no double occupancy and it is highly degenerate since the spins can take any orientation. Hopping will split this degeneracy. Let us write the eigenvalue problem for the Hubbard Hamiltonian in the block form

$$\left(\begin{array}{cc} H_{11} & H_{12} \\ H_{21} & H_{22} \end{array} \right) \left(\begin{array}{c} X \\ Y \end{array} \right) = E \left(\begin{array}{c} X \\ Y \end{array} \right) \tag{1.78}$$

where H_{11} contains only terms that stay within the singly occupied subspace, H_{12} and H_{21} contains hopping that links the singly occupied subspace with the other ones and H_{22} contains terms that connect states where there is double occupancy. Formally, this separation can be achieved using projection operators. To project a state in the singly occupied subspace, one uses $H_{11} = PHP$ where the projector P is

$$P = \prod_{i=1}^{N} (1 - n_{i\uparrow} n_{i\downarrow}). \tag{1.79}$$

Returning to the block form of the Hamiltonian, we can solve for $Y = (E - H_{22})^{-1} H_{21} X$ and write

$$\left(H_{11} + H_{12} (E - H_{22})^{-1} H_{21} \right) X = EX. \tag{1.80}$$

What save us here is that the eigenstates we are looking for are near $E = 0$ whereas H_{22} will act on states where there is one singly occupied state since the hopping term in H_{12} can at most create one doubly occupied state from a state with no double occupation. The leading term in H_{22} will thus simbply give a contribution U which is large compared to E. We are left with the eigenvalue problem

$$\left(H_{11} - \frac{H_{12} H_{21}}{U} \right) X = EX. \tag{1.81}$$

The first part of the Hamiltonian H_{11} contains only hopping between states where no site is doubly occupied. The potential energy in those states vanishes.

The quantity $H_{12} H_{21}$ can be computed as follows. The only term of the original Hamiltonian that links singly and doubly occupied states is the hopping part. Let us consider only nearest neighbor hopping with $t_{ij} = -t$. Then

$$H_{12} H_{21} = t^2 \sum_{\langle ij \rangle \sigma} \sum_{\langle kl \rangle \sigma'} \left(c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) \left(c_{k\sigma'}^\dagger c_{l\sigma'} + h.c. \right) \tag{1.82}$$

where each nearest-neighbor bond $\langle ij \rangle$ is counted only once in the sum. Since we leave from a state with singly occupied sites and return to a state with singly occupied sites, $\langle kl \rangle = \langle ij \rangle$ survives as well as cases such as $\langle kl \rangle = \langle il \rangle$ if one of the sites i is empty in the initial state. The latter contribution is called correlated hopping. It describes second-neighbor hopping through a doubly occupied state. In the $t-J$ model, this term is often neglected on the grounds that it is proportional

to t^2/U whereas H_{11} is of order t. That is not necessarily a good reason to neglect this term.

Let us return to the contribution coming from $\langle kl \rangle = \langle ij \rangle$. Discarding terms that destroy two particles on the same site, we are left with only

$$-\frac{H_{12}H_{21}}{U} = -\frac{t^2}{U}\sum_{\langle ij \rangle \sigma\sigma'} \left(c_{i\sigma}^{\dagger}c_{j\sigma}Qc_{j\sigma'}^{\dagger}c_{i\sigma'} + i \leftrightarrow j \right) \qquad (1.83)$$

where Q is the projection operator that makes sure that the intermediate state is doubly occupied. We have to consider four spin configurations for the neighboring sites i and j. The configurations $|i\uparrow\rangle \, |j\uparrow\rangle$ and $|i\downarrow\rangle \, |j\downarrow\rangle$ do not contribute since the intermediate state is prohibited by the Pauli principle. The configuration $|i\uparrow\rangle \, |j\downarrow\rangle$ when acted upon by the first term in the last equation Eq.(1.83) has non-zero matrix elements with two possible finite states, $\langle i\uparrow| \langle j\downarrow|$ and $\langle i\downarrow| \langle j\uparrow|$. The matrix element has the value $-t^2/U$ for the first case and t^2/U for the configuration where the spins have been exchanged because of the fermionic nature of the states. The configuration $|i\downarrow\rangle \, |j\uparrow\rangle$ has the corresponding possible final states. And the $i \leftrightarrow j$ term in Eq.(1.83) just doubles the previous results, in other words the magnitude of the non-zero matrix elements is $2t^2/U$. Since only spins are involved, all we need to do is to find spin operators that have exactly the same matrix elements.

What we are looking for is

$$\frac{4t^2}{U\hbar^2}\sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{\hbar^2}{4}n_in_j \right) = J\sum_{\langle ij \rangle} \left(S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+ \right) - \frac{\hbar^2}{4}n_in_j \right) \qquad (1.84)$$

where $J \equiv 4t^2/U\hbar^2$. Indeed, if the neighboring spins are parallel, the quantity $S_i^+ S_j^- + S_i^- S_j^+$ has zero expectation value while the expectation of $S_i^z S_j^z$, namely $\hbar^2/4$, is cancelled by the expectation of $-\hbar^2 n_in_j/4$. For antiparallel spins, $S_i^z S_j^z - \hbar^2 n_in_j/4$ has expectation value $-\hbar^2/2$ between configurations where the spins do not flip while $\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+ \right)$ has vanishing matrix elements. In the case where the spins flip between the initial and final state, only $\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+ \right)$ has non-zero expectation value and it is equal to $\hbar^2/2$. With the definition of J given, this corresponds to the matrix elements we found above.

This is the form of the Heisenberg Hamiltonian. Including the correlated hopping term, the $t-J$ Hamiltonian takes the following form

$$H = P\left[\sum_{\langle ij \rangle \sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma} + J\sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{\hbar^2}{4}n_in_j \right)\right]P \qquad (1.85)$$

$$+P\left[-\frac{J}{4}\sum_{i,k\neq k'} \left(c_{i,-\sigma}^{\dagger}c_{j,-\sigma}c_{j+k,\sigma}^{\dagger}c_{j+k',\sigma} + c_{j+k,-\sigma}^{\dagger}c_{i,-\sigma}^{\dagger}c_{j,-\sigma}c_{j+k',\sigma} \right)\right]P$$

where the last term is the three-site hopping term that is usually neglected.

It is remarkable, but expected, that at half-filling the effective Hamiltonian is a spin-only Hamiltonian (The first term in the above equation does not contribute when there is no hole because of the projection operators). From the point of view of perturbation theory, the potential energy is the large term. We are in an insulating phase and hopping has split the spin degeneracy.

Classically, the ground state on a hypercubic lattice would be an antiferromagnet. This mechanism for antiferromagnetism is known as *superexchange*.

In closing, one should remember that to compute the expectation value of any operator in the singly occupied space, one must first write it in block form, in other

words, one should not forget the contribution from the Y component of the wave function. *For example, the kinetic energy $\langle K \rangle$ of the Hubbard model calculated in the low energy subspace will be equal to minus twice the potential energy $\langle V \rangle$.* That can be seen from

$$\langle K \rangle \quad = \quad (X \; Y) \, K \begin{pmatrix} X \\ Y \end{pmatrix} = (XKY) + (YKX) = -\frac{2}{U} \, (X \; KK \; X) \tag{1.86}$$

$$\langle V \rangle \quad = \quad (X \; Y) \, V \begin{pmatrix} X \\ Y \end{pmatrix} = (YVY) = +\frac{1}{U} \, (X \; KK \; X) \tag{1.87}$$

since in the intermediate state, V gives the eigenvalue U in all intermediate states.

1.5.3   Anderson lattice model

In the Anderson lattice model, on purely phenomenological grounds one considers localized states $\left(f_{i\sigma}^{\dagger} \right)$ with a Hubbard U, hybridized with a conduction band $\left(c_{\mathbf{k}\sigma}^{\dagger} \right)$ of non-interacting electrons. This model is particularly useful for heavy fermions, for example, where one can think of the localized states as being f electrons:

$$H_A \quad = \quad H_f + H_c + H_{fc} \tag{1.88}$$

$$H_f \quad \equiv \quad \sum_{\sigma} \sum_{i} \varepsilon f_{i\sigma}^{\dagger} f_{i\sigma} + \sum_{i} U \left(f_{i\uparrow}^{\dagger} f_{i\uparrow} \right) \left(f_{i\downarrow}^{\dagger} f_{i\downarrow} \right) \tag{1.89}$$

$$H_c \quad \equiv \quad \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \tag{1.90}$$

$$H_{fc} \quad \equiv \quad \sum_{\sigma} \sum_{i} V_i c_{i\sigma}^{\dagger} f_{i\sigma} + h.c. \tag{1.91}$$

In the case where there is only one site with f electrons, one speaks of the Anderson impurity model. When U is large, one can proceed as for the $t-J$ Hamiltonian and obtain an effective model where there is no double occupancy of the impurity and where the spin of the conduction electrons interacts with the spin of the impurity. The transformation is called the Schrieffer-Wolf transformation and the effective Hamiltonian is the Kondo Hamiltonian.

1.6   Broken symmetry and canonical transformations

The occurence of broken symmetry can be obtained from mathematical arguments only in very few situations, such as the Ising model in two dimensions. A simple paramagnetic state and a state with broken symmetry are separated by a phase transition, in other words by singularities in the free energy. Hence, the broken symmetry state cannot be obtained perturbatively. One postulates a one-body Hamiltonian where the symmetry is broken its stability verified using variational arguments. In this and many other contexts, canonical transformations are key tools to understand and solve the problem. We have seen examples above. Basis changes obtained from unitary transformations preserve the (anti)commutation relations. Such transformations are called canonical. We will illustrate these concepts with the example of superconductivity.

1.6.1 The BCS Hamiltonian

The general idea of Cooper pairs is that $c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}$ almost plays the role of a boson $b^\dagger_{\mathbf{p}}$. Commutation relations are not the same, but we want to use the general idea that superconductivity will be described by a non-zero expectation value of $b^\dagger_{\mathbf{p}}$ by analogy to superfluidity. The expectation value $\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle$ occurs in the Ginzburg-Landau theory as a pair wave function. The mean-field state will be described by a coherent state.

We first write the general Hamiltonian in momentum space and, in the spirit of Weiss, the trial Hamiltonian for the mean-field takes the form

$$
\begin{aligned}
H_E - \mu N &= H_0 - \mu N + \frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'} U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\right\rangle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\\
&\quad + \frac{1}{V}\sum_{\mathbf{p},\mathbf{p}'} U\left(\mathbf{p}-\mathbf{p}'\right) c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle\\
&= H_0 - \mu N + \sum_{\mathbf{p}}\left(\Delta^*_{\mathbf{p}}c_{-\mathbf{p}\downarrow}c_{\mathbf{p}\uparrow} + c^\dagger_{\mathbf{p}\uparrow}c^\dagger_{-\mathbf{p}\downarrow}\Delta_{\mathbf{p}}\right) \qquad (1.92)
\end{aligned}
$$

where we defined

$$
\Delta_{\mathbf{p}} = \frac{1}{V}\sum_{\mathbf{p}'} U\left(\mathbf{p}-\mathbf{p}'\right)\left\langle c_{-\mathbf{p}'\downarrow}c_{\mathbf{p}'\uparrow}\right\rangle. \qquad (1.93)
$$

The potential $U\left(\mathbf{p}-\mathbf{p}'\right)$ is an effective attraction that comes from phonons in standard BCS theory. We take this for granted. The states within an energy shell of size $\hbar\omega_D$ around the Fermi level are those that are subject to that attraction. The kinetic part of the Hamiltonian is given by

$$
\begin{aligned}
H_0 - \mu N &= \sum_{\mathbf{p},\sigma}\left(\varepsilon_{\mathbf{p}}-\mu\right)c^\dagger_{\mathbf{p},\sigma}c_{\mathbf{p},\sigma} \qquad (1.94)\\
&\equiv \sum_{\mathbf{p},\sigma}\zeta_{\mathbf{p}}c^\dagger_{\mathbf{p},\sigma}c_{\mathbf{p},\sigma}. \qquad (1.95)
\end{aligned}
$$

In the so-called jellium model, $\varepsilon_{\mathbf{p}} = \hbar^2\mathbf{p}^2/2m_e$ but one can take a more general dispersion relation. In matrix form, the combination of all these terms gives, within a constant

$$
H_E - \mu N = \sum_{\mathbf{p}}\begin{pmatrix} c^\dagger_{\mathbf{p}\uparrow} & c_{-\mathbf{p}\downarrow} \end{pmatrix}\begin{pmatrix} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta^*_{\mathbf{p}} & -\zeta_{-\mathbf{p}} \end{pmatrix}\begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix}. \qquad (1.96)
$$

One is looking for a canonical transformation that diagonalize the Hamiltonian. When this will be done, the $c^{(\dagger)}_{-\mathbf{p}\downarrow}$ will be linear combinations of eigenoperators. These linear combinations will involve $\Delta_{\mathbf{p}}$. To find the value of $\Delta_{\mathbf{p}}$, it will suffice to substitute the eigenoperator expression for $c_{\mathbf{p}\sigma}$ in the definition of $\Delta_{\mathbf{p}}$, Eq.(1.93). This will give a self-consistent expression for $\Delta_{\mathbf{p}}$.

Let us define the Nambu spinor

$$
\Psi_{\mathbf{p}} = \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c^\dagger_{-\mathbf{p}\downarrow} \end{pmatrix} \qquad (1.97)
$$

whose anticommutator is

$$
\left\{\Psi_{\mathbf{p},i}, \Psi^\dagger_{\mathbf{p}',j}\right\} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{i,j} \qquad (1.98)
$$

where i and j identibly the components of the Nambu spinor. Any unitary transformation of the Nambu spinors will satisfy the anticommutation relations, as one can easily check. Since the Hamiltonian matrix is Hermitian, it can be diagonalized by a unitary transformation.

Eigenvalues $E_{\mathbf{p}}$ are obtained from the characteristic equation

$$\left(\lambda_{\mathbf{p}} - \zeta_{\mathbf{p}}\right)\left(\lambda_{\mathbf{p}} + \zeta_{\mathbf{p}}\right) - |\Delta_{\mathbf{p}}|^2 = 0 \tag{1.99}$$

where one used $\zeta_{\mathbf{p}} = \xi_{-\mathbf{p}}$ valid for a lattice with inversion symmetry. The solutions are

$$\lambda_{\mathbf{p}} = \pm E_{\mathbf{p}} = \pm\sqrt{\zeta_{\mathbf{p}}^2 + |\Delta_{\mathbf{p}}|^2} \tag{1.100}$$

and the eigenvectors obey

$$\left(\begin{array}{cc} \pm E_{\mathbf{p}} - \zeta_{\mathbf{p}} & -\Delta_{\mathbf{p}} \\ -\Delta_{\mathbf{p}}^* & \pm E_{\mathbf{p}} + \zeta_{\mathbf{p}} \end{array}\right)\left(\begin{array}{c} a_{1\mathbf{p}} \\ a_{2\mathbf{p}} \end{array}\right) = 0. \tag{1.101}$$

whose solution is

$$\left(\pm E_{\mathbf{p}} - \zeta_{\mathbf{p}}\right) a_{1\mathbf{p}} = \Delta_{\mathbf{p}} a_{2\mathbf{p}} \tag{1.102}$$

The constraint of normalization for a unitary transformation is

$$|a_{1\mathbf{p}}|^2 + |a_{2\mathbf{p}}|^2 = 1. \tag{1.103}$$

The unitary transformation U

$$U = \left(\begin{array}{cc} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v_{\mathbf{p}}^* & u_{\mathbf{p}}^* \end{array}\right) \tag{1.104}$$

$$U^\dagger = \left(\begin{array}{cc} u_{\mathbf{p}}^* & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^* & u_{\mathbf{p}} \end{array}\right) \tag{1.105}$$

where

$$\left(\begin{array}{c} u_{\mathbf{p}} \\ v_{\mathbf{p}}^* \end{array}\right) = \frac{1}{\sqrt{2}}\left(\begin{array}{c} \left(1 + \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{-i\phi_{1\mathbf{p}}} \\ \left(1 - \frac{\zeta_{\mathbf{p}}}{E_{\mathbf{p}}}\right)^{1/2} e^{i\phi_{2\mathbf{p}}} \end{array}\right)$$

diagonalizes the Hamiltonian

$$\left(\begin{array}{cc} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{array}\right) = U^\dagger \left(\begin{array}{cc} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^* & -\zeta_{\mathbf{p}} \end{array}\right) U.$$

Using this result, we can write

$$H_E - \mu N = \sum_{\mathbf{p}} \left(\begin{array}{cc} c_{\mathbf{p}\uparrow}^\dagger & c_{-\mathbf{p}\downarrow} \end{array}\right) U U^\dagger \left(\begin{array}{cc} \zeta_{\mathbf{p}} & \Delta_{\mathbf{p}} \\ \Delta_{\mathbf{p}}^* & -\zeta_{\mathbf{p}} \end{array}\right) U U^\dagger \left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{array}\right) \tag{1.106}$$

$$= \sum_{\mathbf{p}} \left(\begin{array}{cc} \alpha_{\mathbf{p}\uparrow}^\dagger & \alpha_{-\mathbf{p}\downarrow} \end{array}\right) \left(\begin{array}{cc} E_{\mathbf{p}} & 0 \\ 0 & -E_{\mathbf{p}} \end{array}\right) \left(\begin{array}{c} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^\dagger \end{array}\right) \tag{1.107}$$

$$= \sum_{\mathbf{p},\sigma} E_{\mathbf{p}} \alpha_{\mathbf{p},\sigma}^\dagger \alpha_{\mathbf{p},\sigma} + cte. \tag{1.108}$$

where the new operators are related to the old by the Bogoliubov-Valentin (1958) transformation

$$\left(\begin{array}{c} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^\dagger \end{array}\right) = U^\dagger \left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{array}\right) = \left(\begin{array}{cc} u_{\mathbf{p}}^* & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^* & u_{\mathbf{p}} \end{array}\right) \left(\begin{array}{c} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{array}\right). \tag{1.109}$$

The ground state is the state that is annihilated by these new operators

$$\alpha_{\mathbf{p}\sigma} |BCS\rangle = 0.$$

The new operators are linear combination of creation-annihilation operators since the eigenstate is a linear combination of states having different numbers of particles. At zero temperature for example, one can check explicitly that the following state is indeed annihilated by $\alpha_{\mathbf{p}\sigma}$

$$|BCS\rangle = \prod_{\mathbf{k}} \left(1 + \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^*} c_{-\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger \right) |0\rangle.$$

The value of the gap $\Delta_{\mathbf{p}}$ is obtained from the self-consistency equation Eq.(1.93). It suffices to write the $c_{\mathbf{p}\uparrow}$ en as a function of the diagonal operators $\alpha_{\mathbf{p}\sigma}$. Inverting the Bogoliubov transformation Eq.(1.109) gives

$$\begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{p}} & -v_{\mathbf{p}} \\ v_{\mathbf{p}}^* & u_{\mathbf{p}}^* \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{p}\uparrow} \\ \alpha_{-\mathbf{p}\downarrow}^\dagger \end{pmatrix} \tag{1.110}$$

whose adjoint is

$$\begin{pmatrix} c_{\mathbf{p}\uparrow}^\dagger & c_{-\mathbf{p}\downarrow} \end{pmatrix} = \begin{pmatrix} \alpha_{\mathbf{p}\uparrow}^\dagger & \alpha_{-\mathbf{p}\downarrow} \end{pmatrix} \begin{pmatrix} u_{\mathbf{p}}^* & v_{\mathbf{p}} \\ -v_{\mathbf{p}}^* & u_{\mathbf{p}} \end{pmatrix}. \tag{1.111}$$

We also note that

$$n(E_{\mathbf{p}}) \equiv \left\langle \alpha_{\mathbf{p}\uparrow}^\dagger \alpha_{\mathbf{p}\uparrow} \right\rangle = \frac{1}{e^{\sigma' E_{\mathbf{p}}} + 1}. \tag{1.112}$$

The Fermi-Dirac distribution arises from the fact the the Hamiltonian is diagonal and quadratic when written as a function of fermionic operators $\alpha_{\mathbf{p}}^{(\dagger)}$. We can now compute the mean value of the pair operator.

$$\begin{aligned}
\langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle &= \left\langle \left(v_{\mathbf{p}'} \alpha_{\mathbf{p}'\uparrow}^\dagger + u_{\mathbf{p}'} \alpha_{-\mathbf{p}'\downarrow} \right) \left(u_{\mathbf{p}'} \alpha_{\mathbf{p}'\uparrow} - v_{\mathbf{p}'} \alpha_{-\mathbf{p}'\downarrow}^\dagger \right) \right\rangle & (1.113) \\
&= v_{\mathbf{p}'} u_{\mathbf{p}'} \left\langle \alpha_{\mathbf{p}'\uparrow}^\dagger \alpha_{\mathbf{p}'\uparrow} - \alpha_{-\mathbf{p}'\downarrow} \alpha_{-\mathbf{p}'\downarrow}^\dagger \right\rangle & (1.114) \\
&= -v_{\mathbf{p}'} u_{\mathbf{p}'} \left(1 - 2n(E_{\mathbf{p}'}) \right) & (1.115) \\
&= -\frac{1}{2} \left(1 - \frac{\zeta_{\mathbf{p}'}^2}{E_{\mathbf{p}'}^2} \right)^{1/2} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2n(E_{\mathbf{p}'}) \right) & (1.116) \\
&= -\frac{1}{2} \frac{|\Delta_{\mathbf{p}'}|}{E_{\mathbf{p}'}} e^{-i\phi_{1\mathbf{p}'} - i\phi_{2\mathbf{p}'}} \left(1 - 2n(E_{\mathbf{p}'}) \right). & (1.117) \\
&= -\frac{1}{2} \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n(E_{\mathbf{p}'}) \right) & (1.118)
\end{aligned}$$

Substituting in self-consistency equation, we Eq.(1.93) on obtain

$$\Delta_{\mathbf{p}} = -\frac{1}{2V} \sum_{\mathbf{p}'} U(\mathbf{p} - \mathbf{p}') \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \left(1 - 2n(E_{\mathbf{p}'}) \right). \tag{1.119}$$

where $\Delta_{\mathbf{p}}$ is in general complex. This is known as the BCS equation.

Remark 3 *Even when the interaction depends on $\mathbf{p} - \mathbf{p}'$, the phase is necessarily independent of $\mathbf{p}$. Indeed, the gap equation can be rewritten in the form*

$$[C_{\mathbf{p}} \Delta_{\mathbf{p}}] = -\frac{1}{2V} \sum_{\mathbf{p}'} C_{\mathbf{p}} U(\mathbf{p} - \mathbf{p}') C_{\mathbf{p}'} [C_{\mathbf{p}'} \Delta_{\mathbf{p}'}]. \tag{1.120}$$

where

$$C_{\mathbf{p}} = \left(\frac{(1 - 2n\,(E_{\mathbf{p}}))}{E_{\mathbf{p}}} \right)^{1/2}. \tag{1.121}$$

The gap equation can then be reinterpreted as an eigenvalue equation. The eigenvectors are in brackets and the eigenvalue is unity. Since the matrix $-C_{\mathbf{p}}U\,(\mathbf{p} - \mathbf{p}')\,C_{\mathbf{p}'}/\,(2V)$ whose eigenvalues we are looking for is real and symmetric, the eigenvector is real within a global phase, i.e. a complex number $e^{i\phi}$ that multiplies all components of the eigenvector. This independence of $\mathbf{p}$ of the phase is known as "phase coherence". It is key to superconductivity, If the eigenvalue of the gap equation is degenerate, something new can happen. One obvious degeneracy is associated with time-reversal symmetry. When this symmetry is broken, there is still an overall $\mathbf{p}$ independent phase, but the order parameter is complex in a way that does not correspond to a global phase. This in general gives, for example, a non-trivial value of the orbital angular momentum.

Remark 4 *Coherence: Since $\phi_{1\mathbf{p}} + \phi_{2\mathbf{p}} = \phi$ for all values of $\mathbf{p}$, all the pairs are added to the wave function with exactly the same phase. This can be seen from the BCS wave function at zero temperature*

$$\prod_{\mathbf{k}} \left(1 + \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^*} c_{-\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger \right) |0\rangle.$$

It is the interactions that impose that phase coherence that is at the origin of the phenomenon of superconductivity. Only the overall $\mathbf{p}$ independent phase of Δ is arbitrary. The global gauge symmetry is broken by fixing the phase since phase and number obey an uncertainty relation. Fixing the phase thus corresponds to making the total number of particles uncertain.

1.7 Elementary quantum mechanics and path integrals

There is one formulation of quantum mechanics that is particularly useful for numerical simulations. It is the path integral formulation. The path integral formulation can be postulated. Quantum mechanics follows. Here we start from more familiar concepts and obtain the path integral formulation, as Feynman did.

Let us go back to a single particle. The amplitude for a particle to go from position x_i to position x_f in a time t is given by

$$G\,(x_f, t; x_i, 0) \equiv \langle x_f |\, e^{-iHt/\hbar}\, |x_i\rangle. \tag{1.122}$$

This amplitude $G\,(x_f, t; x_i, 0)$ is known as the propagator. To simplify the notation we work in one-dimension and we work in units where $\hbar = 1$. It is the basic object of this section.

1.7.1 Physical interpretation of the propagator

There are several ways to physically understand the propagator. From the basic postulates of quantum mechanics, squaring $G\,(x_f, t; x_i, 0)$ gives the probability

that we are in eigenstate of position x_f at time t if the starting state is a position eigenstate x_i. Also, if we know the propagator we know the amplitude to go from any state to any other one. Indeed, inserting complete sets of position eigenstates we find that

$$\langle \psi_f | e^{-iHt/\hbar} | \psi_i \rangle = \int dx_i dx_f \psi_f^* (x_f) \psi_i (x_i) \langle x_f | e^{-iHt} | x_i \rangle \qquad (1.123)$$

Another way to see how to use the propagator is to define the retarded propagator

$$G^R (x_f, t; x_i, 0) \equiv \langle x_f | e^{-iHt} | x_i \rangle \theta (t) \qquad (1.124)$$

where $\theta (t)$ is the heaviside step function. Inserting a complete set of energy eigenstates, we find

$$
\begin{aligned}
G^R (x_f, t; x_i, 0) &\equiv \sum_n \langle x_f | n \rangle e^{-iE_n t} \langle n | x_i \rangle \theta (t) \\
&= \sum_n \phi_n (x_f) \phi_n^* (x_i) e^{-iE_n t} \theta (t) \qquad (1.125)
\end{aligned}
$$

The Fourier transform of this quantity with η a positive real number is

$$\int_{-\infty}^{\infty} dt e^{i(z+i\eta)t} G^R (x_f, t; x_i, 0) = i \sum_n \frac{\phi_n (x_f) \phi_n^* (x_i)}{z + i\eta - E_n}. \qquad (1.126)$$

The poles of this function give the eigenenergies and the residues are related to the wave functions. In the many-body context, a generalization of the propagator occurs very naturally in perturbation theory.

In statistical physics, $\langle x_f | \rho | x_i \rangle$ is a quantity of interest. Using the known form of the density matrix, we have $\langle x_f | \rho | x_i \rangle = \langle x_f | e^{-\beta H} | x_i \rangle / Z$. Hence, computing these matrix elements is like computing the propagator in imaginary time τ with the substitution $t \to -i\tau$. This analogy holds also in the many-bady context.

1.7.2 Computing the propagator with the path integral

In general, H contains non-commuting pieces. The potential energy V is diagonal in position space, but the kinetic energy K is diagonal in momentum space. Hence, computing the action of e^{-iHt} on $|x_i\rangle$ is non-trivial since we need to diagonalize the Hamiltonian to compute the value of the exponential of an operator and that Hamiltonian contains two non-commuting pieces that are diagonal in different basis. The key observation is that if the time interval t is very small, say ε, then the error that we do in writing the exponential as a product of exponentials is of order ε^2 since it depends on the commutator of $K\varepsilon$ with $V\varepsilon$

$$e^{-iH\varepsilon} \sim e^{-iK\varepsilon} e^{-iV\varepsilon} + O\left(\varepsilon^2\right). \qquad (1.127)$$

In fact the error of order ε^2 is in the argument of the exponential, as one can see from the Baker-Campbell-Hausdorff formula $e^A e^B = e^M$ with

$$M = A + B + \frac{1}{2} [A, B] + a_2 [A, [A, B]] + \dots \qquad (1.128)$$

In numerical calculations it is important to keep the exponential form since this garantees unitarity.

Other factorizations give errors of even higher order. For example,

$$e^{-iH\varepsilon} \sim e^{-iV\varepsilon/2}e^{-iK\varepsilon}e^{-iV\varepsilon/2} \tag{1.129}$$

gives an error of order ε^3. In practice, for numerical simulations it is quite useful to use factorizations that lead to higher order errors. To continue analytically however, the simplest factorization suffices.

In the factorized form, we can take advantage of the fact that we can introduce complete sets of states where the various pieces of the Hamiltonian are diagonal to compute the propagator for an infinitesimal time

$$\langle x_f | e^{-iK\varepsilon}e^{-iV\varepsilon} | x_i \rangle = \int \frac{dp}{2\pi} \langle x_f | e^{-iK\varepsilon} | p \rangle \langle p | e^{-iV\varepsilon} | x_i \rangle \tag{1.130}$$

$$= \int \frac{dp}{2\pi} e^{i\left[-\varepsilon\frac{p^2}{2m} + p(x_f - x_i) - \varepsilon V(x_i)\right]} \tag{1.131}$$

where we used $\langle x | p \rangle = e^{ipx}$. The last formula can be rewritten

$$\int \frac{dp}{2\pi} e^{i(p\dot{x} - H)\varepsilon} \tag{1.132}$$

where

$$\dot{x} \equiv \frac{x_f - x_i}{\varepsilon}. \tag{1.133}$$

The argument of the exponential is the Lagrangian times the time interval. It thus has the units of action and is made dimensionless by dividing by the quantum of action $\hbar$ that we have set to unity.

For a finite time interval, we simply split the time evolution operator into evolution pieces that involve over an infinitesimal time interval

$$e^{-iHt} = \prod_{i=1}^{N} e^{-iH\varepsilon} \tag{1.134}$$

where $\varepsilon = t/N$. There is no approximation here. Inserting $N-1$ complete sets of states, we have

$$\langle x_f | e^{-iHt} | x_i \rangle = \int \prod_{j=1}^{N-1} dx_j \langle x_f | e^{-iH\varepsilon} | x_{N-1} \rangle \langle x_{N-1} | e^{-iH\varepsilon} | x_{N-2} \rangle \langle x_2 | \dots$$

$$| x_1 \rangle \langle x_1 | e^{-iH\varepsilon} | x_i \rangle . \tag{1.135}$$

Each of the N matrix elements can be evaluated now using the previous trick so that the propagator is given by the formally exact expression

$$\langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \int \prod_{j=1}^{N-1} dx_j \int \prod_{j=1}^{N} dp_j \exp\left[i \left(p_N \frac{x_f - x_{N-1}}{\varepsilon} - \frac{p_N^2}{2m} - V(x_{N-1}) \right) \varepsilon \right.$$

$$+ i \left(p_{N-1} \frac{x_{N-1} - x_{N-2}}{\varepsilon} - \frac{p_{N-1}^2}{2m} - V(x_{N-2}) \right) \varepsilon$$

$$+ \dots$$

$$\left. + i \left(p_1 \frac{x_1 - x_i}{\varepsilon} - \frac{p_1^2}{2m} - V(x_i) \right) \varepsilon \right] \tag{1.136}$$

To do the calculation, this is what one has to do. Formally however, the final expression is quite nice. It can be written as a path integral in phase space

$$\langle x_f | e^{-iHt} | x_i \rangle = \int [DxDp] \exp\left\{ i \int dt \, [p\dot{x} - H(p,x)] \right\} \tag{1.137}$$

$$= \int [DxDp] \exp iS(x,p) \tag{1.138}$$

where the definition of the measure $[Dx Dp]$ is clear by comparison and where S is the action.

It is more natural to work in configuration space where the Lagrangian is normally defined. This comes out automatically by doing the integral over all the intermediate momenta. They can be done exactly since they are all Gaussian integrals that are easily obtained by completing the square

$$
\int \frac{dp}{2\pi} \exp i \left(p_{N-1} \frac{x_{N-1} - x_{N-2}}{\varepsilon} - \frac{p_{N-1}^2}{2m} \right) \varepsilon = \sqrt{\frac{m}{2\pi i \varepsilon}} \exp \left[\frac{im}{2} \left(\frac{x_{N-1} - x_{N-2}}{\varepsilon} \right)^2 \varepsilon \right]
$$

$$
= \sqrt{\frac{m}{2\pi i \varepsilon}} \exp \left[\frac{im}{2} \dot{x}_{N-1}^2 \varepsilon \right]. \qquad (1.139)
$$

Remark 5 *The above is the propagator for a free particle. In that case, the time interval could be arbitrary and the result could also be obtained using our earlier decomposition on energy eigenstates since*

$$
\sum_n \phi_n (x_f) \phi_n^* (x_i) e^{-iE_n t} = \int \frac{dp}{2\pi} e^{ip(x_f - x_i) - it \frac{p^2}{2m}}. \qquad (1.140)
$$

Once the integrals over momenta have been done, we are left with

$$
\langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \int \prod_{j=1}^{N-1} dx_j \left(\sqrt{\frac{mN}{2\pi i t}} \right)^N \exp \left[i\varepsilon \left(\frac{m}{2} \left(\frac{x_f - x_{N-1}}{\varepsilon} \right)^2 - V \left(x_{N-1} \right) \right) \right.
$$

$$
+ i\varepsilon \left(\frac{m}{2} \left(\frac{x_{N-1} - x_{N-2}}{\varepsilon} \right)^2 - V \left(x_{N-2} \right) \right)
$$

$$
+ \ldots
$$

$$
\left. + i\varepsilon \left(\frac{m}{2} \left(\frac{x_1 - x_i}{\varepsilon} \right)^2 - V \left(x_i \right) \right) \right] \qquad (1.141)
$$

$$
= \int_{x_i}^{x_f} Dx \exp \left(i \int_0^t dt' \left(\frac{1}{2} m \dot{x}^2 - V (x) \right) \right) = \int_{x_i}^{x_f} Dx e^{iS(\dot{x}, x)} \qquad (1.142)
$$

where the formal expression makes clear only that it is the integral of the Lagrangian, hence the action, that comes in the argument of the exponential. The integration measure here is different from the one we had before. This form is particularly useful for statistical physics where all the integrals are clearly convergent, as opposed to the present case where they oscillate rapidly and do not always have a clear meaning.

The physical interpretation of this result is quite interesting. It says that the amplitude for going from one point to another in a given time is given by the sum amplitydes for all possible ways of going between these two points in the given time, each path, or trajectory, being weighted by an exponential whose phase is the classical action measured in units of the action quantum $\hbar$. The classical limit is obtained when the action is large compared with the quantum of action. Indeed, in that case the integral can be evaluated in the stationary phase approximation. In that approximation, one expands the action to quadratic order around the trajectory that minimizes the action. That trajectory, given by the Euler-Lagrange equation, is the classical trajectory according to the principle of least action.

Remark 6 *The exponentials in the path integral are time-ordered, i.e. the ones correspondint to later times are always to the left of those with earlier times. This time-ordering feature will be very relevant later for Green functions.*

1.7.3 Coherent-state path integrals

In the many-body context, the amplitudes that are interesting are of the form

$$\mathrm{Tr}\left[\rho c_f\left(t\right)c_i^\dagger\right].\tag{1.143}$$

In the special case where only the ground state contibutes and that state is the vacuum state (i.e. no particle present), the above reduces precisely to our previous definition since $c_i^\dagger\left|0\right\rangle = \left|x_i\right\rangle$ and $\left\langle 0\right|e^{-\beta H}c_f\left(t\right) = \left\langle 0\right|e^{-\beta H}e^{iHt}c_f e^{-iHt} = \left\langle 0\right|c_f e^{-iHt} = \left\langle x_f\right|e^{-iHt}$.

To derive a path integral formulation for that type of amplitude, we note that destruction operators in H always appear first on the right. Hence, if we replace the position eigenstates in the one-particle case by eigenstates of the destruction operator, we will be able to derive a path integral formulation in the many-body case by following an analogous route. We will not do the full derivation here. The final result is that both for bosons and fermions, the path integral also involves exponentials of the action. For fermions, one must introduce Grassmann algebra with non-commuting numbers to define coherent states. For bosons the situation is simpler.

Let us see how boson coherent states are constructed. Let $\left[a,a^\dagger\right] = 1$, then define the coherent state $\left|z\right\rangle$ by

$$\left|z\right\rangle = e^{-|z|^2/2}e^{za^\dagger}\left|0\right\rangle.\tag{1.144}$$

To show that this is an eigenstate of a, note first that one can easily show by induction that

$$\left[a,\left(a^\dagger\right)^n\right] = n\left(a^\dagger\right)^{n-1}\tag{1.145}$$

which formally looks like

$$\left[a,\left(a^\dagger\right)^n\right] = \frac{\partial\left(a^\dagger\right)^n}{\partial a^\dagger}\tag{1.146}$$

and since the exponential is defined in terms of its power series

$$\left[a,e^{za^\dagger}\right] = \frac{\partial e^{za^\dagger}}{\partial a^\dagger} = ze^{za^\dagger}\tag{1.147}$$

Using our little theorem on commutators of ladder operators (1.3.2), we have that since $a\left|0\right\rangle = 0$ then $a\left(e^{za^\dagger}\left|0\right\rangle\right) = z\left(e^{za^\dagger}\left|0\right\rangle\right)$ and $\left|z\right\rangle$ is an eigenstate of a.

To show that $\left|z\right\rangle$ is normalized, consider

$$\begin{aligned}\left\langle z\mid z\right\rangle &= e^{-|z|^2}\left\langle 0\right|e^{z^*a}e^{za^\dagger}\left|0\right\rangle = e^{-|z|^2}e^{|z|^2}\left\langle 0\right|e^{za^\dagger}\left|0\right\rangle\\&= 1\end{aligned}\tag{1.148}$$

In the last step, one has simply expanded the exponential in a power series and used the normalization of the vacuum.

Finally we the closure relation

$$I = \frac{1}{\pi}\int dz\,dz^*\left|z\right\rangle\left\langle z\right|\tag{1.149}$$

that can be proven by taking matrix elements with states with arbitrary number of bosons $\left|n\right\rangle = \left(a^\dagger\right)^n\left|0\right\rangle/\sqrt{n!}$ and doing the integral in polar coordinates.

2. RESPONSE FUNCTIONS AND THEIR GENERAL PROPERTIES

Whether perturbation theory is applicable or not, we rarely need all the information contained in the wave-function. A reduced description in terms of only a few variables suffices if it allows us to explain what can be observed by experimental probes. Correlation functions offer us such a description. As for any physical theory, we thus first discuss which quantities are observable, or in other words, what it is that we want to compute.

Whatever the appropriate microscopic description of the system, or whatever the underlying broken symmetry, the result of any given type of experiment can be expressed as a specific correlation function.

We will need to treat two different aspects of correlation functions.

First, general properties, which are independent from the specific manner in which we compute correlation functions. For example

- Symmetries

- Positivity

- Fluctuation-dissipation theorems relating linear response and equilibrium fluctuations

- Kramers-Kronig transformations, which follow from causality

- Kubo relations, such as that relating linear response to a specific correlation function.

- Sum rules

- Goldstone theorem, which follows from Bogoliubov inequalities

Second, we will need to develop techniques to compute specific correlation functions. Sometimes, phenomenological considerations suffice to find, with unknown parameters, the functional dependence of correlations functions on say wave-vector and frequency. These phenomenological considerations apply in particular in the hydrodynamic regime, and whenever projection operator techniques are used.

Microscopic approaches will lead us to use another type of correlation functions, namely Green's functions. In fact, Green's function are just one type of correlation function. They will appear very naturally. Furthermore, many of the general properties of correlation functions which we discuss in the present chapter will transpose directly to these functions. Much of this section is inspired from Foster.[1]

In the present chapter, we intend to

- Recall that scattering experiments are a measure of equilibrium fluctuations

- Linear response to an external perturbation can be expressed as an equilibrium correlation function

And this correlation function can be related to equilibrium fluctuations by the fluctuation-dissipation theorem.

- Then we discuss general properties of correlation functions

- Give a specific example of sum-rule calculation.

2.1 Relation between correlation functions and experiments

Scattering experiments with weak probes usually measure various equilibrium correlation functions of a system. What we mean by "weak probes" is simply that Fermi's Golden rule and the Born approximation are all that we need to describe the effect of the system on the external probe, and vice-versa. As an example, consider inelastic electron scattering but it should be clear that similar considerations apply to a large number of cases: inelastic light scattering, neutron scattering, etc...

The plan is simply to use Fermi's Golden Rule to compute the cross section. One obtains

$$\boxed{\frac{d\sigma}{d\epsilon_f d\Omega_f} = \left[\frac{m^2}{(2\pi)^3 \hbar^5}\frac{k_f}{k_i}\left|V^c_{-\mathbf{q}}\right|^2\right]\int dt\; e^{i\omega t}\left\langle\rho_{\mathbf{q}}(t)\rho_{-\mathbf{q}}(0)\right\rangle} \qquad (2.1)$$

Forgetting for all the details, the key point is that the cross section is related to the Fourier transform of the density-density correlation function. The trick, due to Van Hove, to derive this formula from the Golden rule is to use the Dirac representation of the delta function for energy conservation and the Heisenberg representation to express the final result as a correlation function. Since in the Born approximation, incident and final states of the probe are plane waves, everything about the probe is known. The only reference to it will be through explicitly known matrix elements and quantum numbers, such as momentum, energy, spin etc...

A schematic proof is as follows. From the Golden rule, the transition rate is

$$\frac{2\pi}{\hbar}\sum_{I,F,f}\frac{e^{-\beta E_I}}{Z}\left|\langle F|\langle f|V|I\rangle|i\rangle\right|^2\delta\left(E_F + e_f - E_I - e_i\right) \qquad (2.2)$$

where upper cases refer to the system and lower cases to the probe. The initial and final states can be written as direct product of these since probe and system are far from each other then. We have taken a thermal average over initial states and a sum over all possible final states consistent with energy conservation. The operator V makes the transition. Generally speaking, the operator V takes the form of a product of an operator involving the system, O, times an operator involving the probe o. The product of the densities occurs for example in Coulomb interactions. The previous equation may thus be written as

$$\frac{2\pi}{\hbar}\left|M\right|^2\sum_{I,F}\frac{e^{-\beta E_I}}{Z}\left|\langle F|O|I\rangle\right|^2\delta\left(E_F + e_f - E_I - e_i\right) \qquad (2.3)$$

where $\left|M\right|^2$ involves the probe only. Using the Dirac representation of the delta function and the Heisenberg equations of motion and defining $\hbar\omega = e_f - e_i$ the

energy transfered by the probe to the system, one obtains

$$|M|^2 \sum_{I,F} \int dt e^{-i\left(\frac{E_F - E_i + \hbar\omega}{\hbar}\right)t} \frac{e^{-\beta E_I}}{Z} |\langle F| O |I\rangle|^2 \tag{2.4}$$

$$= |M|^2 \sum_{I} \int dt e^{-i\omega t} \frac{e^{-\beta E_I}}{Z} \langle I| e^{iHt/\hbar} O^\dagger e^{-iHt/\hbar} O |I\rangle \tag{2.5}$$

$$= |M|^2 \sum_{I,F} \int dt e^{-i\omega t} \frac{e^{-\beta E_I}}{Z} \langle I| e^{iHt/\hbar} O^\dagger e^{-iHt/\hbar} |F\rangle \langle F| O |I\rangle \tag{2.6}$$

$$= |M|^2 \sum_{I} \int dt e^{-i\omega t} \frac{e^{-\beta E_I}}{Z} \langle I| e^{iHt/\hbar} O^\dagger e^{-iHt/\hbar} O |I\rangle \tag{2.7}$$

$$= |M|^2 \int dt e^{-i\omega t} \text{Tr} \left[\rho e^{iHt/\hbar} O^\dagger e^{-iHt/\hbar} O \right] \tag{2.8}$$

$$= |M|^2 \int dt e^{-i\omega t} \langle O^\dagger (t) O \rangle . \tag{2.9}$$

The transition rate, from which one deduces cross sections for example, is the Fourier transform of a correlation function.

In the case of photoemission, V is involves the scalar product of the current times the vector potential, which in turn can create or destroy one photon. The latter enters the probe matrix element, as does the creation operator in the current that puts an electron in the final state. The operator O entering the correlation function above is thus the destruction operator. The corresponding correlation function will be related to the Green function as we will see in the next chapter. The Green function is thus a special case of correlation function.

Definition 3 *Note in passing that we use the following definitions for Fourier transforms in the continuum*

$$\boxed{f_{\mathbf{q}} = \int d^3 r \; f(\mathbf{r}) \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}} \tag{2.10}$$

$$\boxed{f(\mathbf{r}) = \int \frac{d^3 k}{(2\pi)^3} f_{\mathbf{q}} \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}} \tag{2.11}$$

$$\boxed{g_\omega = \int dt \; g(t) e^{i\omega t}} \tag{2.12}$$

$$\boxed{g(t) = \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t}} \tag{2.13}$$

2.2 Linear-response theory

We are interested in the response of a system to a weak external perturbation. The electrical conductivity is the response to a weak applied field, the thermal conductivity the response to a thermal gradient etc... The result will be again an equilibrium correlation function. We will be able to relate this correlation function to equilibrium correlation functions of the type just calculated at the end of the last section by developing the so-called "fluctuation-dissipation theorem". The plan to compute the effect of an external perturbation is to add it to the Hamiltonian and then to treat it as a perturbation, taking the full interacting Hamiltonian of the system H_0 as the unperturbed Hamiltonian.

Let

$$\mathcal{H}(t) = H_0 + \delta\mathcal{H}(t) \tag{2.14}$$

where H_0 is the Hamiltonian of the system under study and $\delta\mathcal{H}(t)$ is the perturbation given by the time-dependent Hamiltonian

$$\boxed{\delta\mathcal{H}(t) = -\int d^3 r \, A_i(\mathbf{r}) a_i(\mathbf{r},t).} \tag{2.15}$$

In this expression, A_i is some observable of the system (excluding external perturbation) in the Schrödinger representation, while $a_i(\mathbf{r},t)$ is the external field. Examples of such couplings to external fields include the coupling to a magnetic field $\mathbf{h}$ through the magnetization $\mathbf{M}$, $(A_i(\mathbf{r}) = M_z(\mathbf{r}); \ a_i(\mathbf{r},t) = h_z(\mathbf{r},t))$ or the coupling to an electromagnetic vector potential $\mathbf{A}/c$ through a current $\mathbf{j}$, $(A_i(\mathbf{r}) = j_x(\mathbf{r})\delta_{i,x}; \ a_i(\mathbf{r},t) = A_x(\mathbf{r},t)\delta_{i,x}/c)$ or that of a scalar potential ϕ through the density ρ $(A_i(\mathbf{r}) = \rho(\mathbf{r}); \ a_i(\mathbf{r},t) = \phi(\mathbf{r},t))$. In this approach, it is clear that the external perturbation is represented in the semi-classical approximation, in other words it is not quantized. We first pause to recall the various representations, or pictures, of quantum mechanics, introducing the interaction representation as the framework where perturbation theory is most easily formulated. Then we go on to derive linear response theory.

2.2.1 Schrödinger and Heisenberg pictures

Since the Hamiltonian is the infinitesimal generator of time translations, Schrödinger's equation for a time-dependent Hamiltonian takes the same form as usual,

$$i\hbar\frac{\partial\psi_S}{\partial t} = \mathcal{H}(t)\psi_S. \tag{2.16}$$

Using the fact that $\mathcal{H}(t)$ is Hermitian, one can easily prove that $\partial\langle\psi_S|\psi_S\rangle/\partial t = 0$, in other words that probability is conserved. Hence, the solution of this equation will be given by

$$\psi_S(t) = U(t,t_0)\psi_S(t_0) \tag{2.17}$$

where $U(t,t_0)$ is a unitary operator satisfying

$$U(t_0,t_0) = 1 \tag{2.18}$$

while by time-reversal symmetry

$$U(t_0,t)U(t,t_0) = 1. \tag{2.19a}$$

Conservation of probability gives

$$U(t,t_0)^\dagger U(t,t_0) = 1 \tag{2.20}$$

so that combining the last result with the definition of the inverse, we have,

$$U(t,t_0)^{-1} = U(t,t_0)^\dagger. \tag{2.21}$$

Furthermore, when we can use time-reversal invariance, Eq.(2.19a), we also have

$$U(t,t_0)^{-1} = U(t,t_0)^\dagger = U(t_0,t). \tag{2.22}$$

By definition, for all values of t, the expectation value of an operator is the same in either the Schrödinger, or the Heisenberg picture.

$$\boxed{\langle\psi_S(t)|\mathcal{O}_S|\psi_S(t)\rangle = \langle\psi_H|\mathcal{O}_H(t)|\psi_H\rangle.} \tag{2.23}$$

In the Heisenberg picture the operators are time-dependent while in the Schrödinger picture, only the wave functions are time dependent. Let us choose $t = 0$ to be the time where both representations coincide. The choice of this time is arbitrary, but taking $t = 0$ simplifies greatly the notation. We have then that

$$\mathcal{O}_S(t = 0) = \mathcal{O}_H(t = 0) \equiv \mathcal{O}_S \tag{2.24}$$

$$\psi_S(t = 0) = \psi_H(t = 0) \equiv \psi_S \tag{2.25}$$

Using the expression for the time-dependent wave function, and the equality of matrix elements Eq.(2.23), we obtain

$$\mathcal{O}_H(t) = U^\dagger(t, 0)\mathcal{O}_S U(t, 0). \tag{2.26}$$

One recovers all the usual results for *time-independent* Hamiltonians by noting that in this case, the solution of Schrödinger's equation is,

$$\boxed{U(t, t_0) = e^{-i\mathcal{H}(t - t_0)/\hbar}.} \tag{2.27}$$

Remark 7 *When there is time-reversal invariance, then it is useful to replace the adjoint by the time-reversed operator, so that the connection between Heisenberg and Schrödinger picture Eq.(2.26) becomes*

$$\mathcal{O}_H(t) = U(0, t)\mathcal{O}_S U(t, 0). \tag{2.28}$$

Because we do not want to assume for the time being that there is time-reversal invariance, we shall stick here with the usual expression Eq.(2.26) but in much of the later chapters, the above representation will be used.

2.2.2 Interaction picture and perturbation theory

Perturbation theory is best formulated in the "interaction representation". In this picture, one can think of both operators and wave functions as evolving, as we will see. We take

$$\boxed{\mathcal{H}(t) = H_0 + \delta\mathcal{H}(t)} \tag{2.29}$$

where H_0 is time-independent as above, but the proof can be generalized to time-dependent H_0 simply by replacing $e^{iH_0 t/\hbar}$ everywhere below by the appropriate evolution operator.

The definition of the evolution operator in the interaction representation $U_I(t, 0)$ is given by

$$U(t, 0) \equiv e^{-iH_0 t/\hbar} U_I(t, 0). \tag{2.30}$$

and

$$U(0, t) \equiv U_I(0, t)e^{iH_0 t/\hbar}. \tag{2.31}$$

so that for example

$$\boxed{U(t, t_0) \equiv e^{-iH_0 t/\hbar} U_I(t, t_0)e^{iH_0 t_0/\hbar}} \tag{2.32}$$

We have used the fact that $U_I(t, t_0)$ obeys the same general properties of unitarity as an ordinary evolution operator, as can easily be checked. Again the interaction representation will coincide with the other two at $t = 0$. The justification for the definition of U_I above is that when the external perturbation $\delta\mathcal{H}(t)$ is small,

$U_I(t, t_0)$ is close to unity. If we write again the equality of matrix elements in the general case, we obtain

$$\langle \psi_S(t) | \mathcal{O}_S | \psi_S(t) \rangle = \langle \psi_S | U^\dagger(t, 0) \mathcal{O}_S U(t, 0) | \psi_S \rangle \tag{2.33}$$

$$= \langle \psi_S | U_I^\dagger(t, 0) e^{iH_0 t/\hbar} \mathcal{O}_S e^{-iH_0 t/\hbar} U_I(t, 0) | \psi_S \rangle \tag{2.34}$$

$$= \langle \psi_S | U_I^\dagger(t, 0) \mathcal{O}_I(t) U_I(t, 0) | \psi_S \rangle \tag{2.35}$$

This last result is important. It can be interpreted as saying that the operators in the interaction representation evolve with

$$\boxed{\mathcal{O}_I(t) = e^{iH_0 t/\hbar} \mathcal{O}_S e^{-iH_0 t/\hbar}} \tag{2.36}$$

while the wave functions obey

$$\boxed{|\psi_I(t)\rangle = U_I(t, 0) |\psi_S\rangle} \tag{2.37}$$

In other words, in the interaction picture both the operators and the wave function evolve. We still have to find the equation of motion for $U_I(t, t_0)$. The result will justify why we introduced the interaction representation. Start from Schrödinger's equation,

$$i\hbar \frac{\partial U(t, t_0)}{\partial t} = \mathcal{H}(t) U(t, t_0) \tag{2.38}$$

which gives the equation of motion for $U_I(t, 0)$, namely

$$H_0 e^{-iH_0 t/\hbar} U_I(t, 0) + e^{-iH_0 t/\hbar} i\hbar \frac{\partial}{\partial t} U_I(t, 0) = \mathcal{H}(t) e^{-iH_0 t/\hbar} U_I(t, 0) \tag{2.39}$$

$$i\hbar \frac{\partial}{\partial t} U_I(t, 0) = e^{iH_0 t/\hbar} \delta \mathcal{H}(t) e^{-iH_0 t/\hbar} U_I(t, 0). \tag{2.40}$$

so that using the definition of time evolution of an arbitrary operator in the interaction representation as above (2.36) the equation for the time evolution operator $U_I(t, 0)$ in the interaction representation may be written,

$$i\hbar \frac{\partial}{\partial t} U_I(t, 0) = \delta \mathcal{H}_I(t) U_I(t, 0) \tag{2.41}$$

with the initial condition

$$U_I(0, 0) = 1. \tag{2.42}$$

As expected, Eq.(2.41) tells us that, if there is no perturbation, U_I is equal to unity for all times and only the operators and not the wave function evolve. The interaction representation then reduces to the Heisenberg representation. Multiplying the equation of motion from the right by $U_I(0, t_0)$ we have for an arbitrary initial time

$$\boxed{i\hbar \frac{\partial}{\partial t} U_I(t, t_0) = \delta \mathcal{H}_I(t) U_I(t, t_0)} \tag{2.43}$$

We will come back later to a formal solution of this equation. To linear order in the external perturbation, it is an easy equation to solve by iteration using the initial condition as the initial guess. Indeed, integrating on both sides of the equation of motion (2.43) and using the initial condition, we have

$$\boxed{U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \, \delta \mathcal{H}_I(t') U_I(t', t_0)} \tag{2.44}$$

which, iterated to first order, gives,

$$U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t dt' \, \delta \mathcal{H}_I(t') + \mathcal{O}(\delta \mathcal{H}_I^2) \tag{2.45}$$

and correspondingly

$$U_I^\dagger(t, t_0) = 1 + \frac{i}{\hbar} \int_{t_0}^t dt' \, \delta \mathcal{H}_I(t') + \mathcal{O}(\delta \mathcal{H}_I^2) \tag{2.46}$$

RESPONSE FUNCTIONS AND THEIR GENERAL PROPERTIES

2.2.3 Linear response

Returning to our general considerations, in the case of interest to us the external perturbation in the interaction representation is of the form,

$$\boxed{\delta\mathcal{H}_I(t) = -\int d^3r\, A_i^0(\mathbf{r},t) a_i(\mathbf{r},t)} \tag{2.47}$$

where for short we wrote $A_i^0(\mathbf{r},t)$ to represent a system's observable evolving in the system's Heisenberg representation,

$$A_i^0(\mathbf{r},t) = e^{iH_0 t/\hbar} A_i(\mathbf{r}) e^{-iH_0 t/\hbar}. \tag{2.48}$$

Suppose we want the expectation value of the observable B in the presence of the external perturbation turned on at time t_0. Then, starting from a thermal equilibrium state at time t_0, it suffices to evolve $B(\mathbf{r})$ with the full evolution operator, including the external perturbation.[1]

$$\langle B(\mathbf{r},t)\rangle = \langle U^\dagger(t,t_0) B(\mathbf{r}) U(t,t_0)\rangle \tag{2.49}$$

Using the interaction representation Eq.(2.32), the last equation becomes

$$\langle B(\mathbf{r},t)\rangle = \left\langle U_I^\dagger(t,t_0) B^0(\mathbf{r},t) U_I(t,t_0)\right\rangle. \tag{2.50}$$

In this last expression, $B^0(\mathbf{r},t)$ is now in the system's Heisenberg representation of the system *without the external perturbation*. We also used the fact that $e^{-iH_0 t_0/\hbar}$ commutes with the density matrix and that the trace has a cyclic property to cancel the extra $e^{-iH_0 t_0/\hbar}$ and $e^{iH_0 t_0/\hbar}$ appearing in the equation for the evolution operator in Eq.(2.32).

Using the explicit expression Eq.(2.47) for the external perturbation in the equation for the evolution operator in the interaction representation (2.45), we have that the term linear in applied field is then given by,

$$\delta\langle B(\mathbf{r},t)\rangle = \frac{i}{\hbar}\int_{t_0}^t dt' \int d^3r' \left\langle \left[B^0(\mathbf{r},t), A_i^0(\mathbf{r}',t')\right]\right\rangle a_i(\mathbf{r}',t'). \tag{2.51}$$

It is customary to take $t_0 = -\infty$, assuming that the perturbation is turned-on adiabatically slowly. One then defines a "retarded" response function, or susceptibility χ^R, by

$$\boxed{\delta\langle B(\mathbf{r},t)\rangle = \int_{-\infty}^\infty dt' \int d^3r'\, \chi_{BA_i}^R(\mathbf{r},t;\mathbf{r}',t') a_i(\mathbf{r}',t')} \tag{2.52}$$

with,

$$\boxed{\chi_{BA_i}^R(\mathbf{r},t;\mathbf{r}',t') = \frac{i}{\hbar}\left\langle\left[B^0(\mathbf{r},t), A_i^0(\mathbf{r}',t')\right]\right\rangle \theta(t-t').} \tag{2.53}$$

This response function is called "retarded" because the response always comes after the perturbation, as expected in a causal system. The function $\theta(t-t')$ ensures this causality. One can also define anti-causal response functions. We come back to this later. For the moment, recall that the superscript 0 here means to zeroth order in the external probe. In other words, the linear response is given by an equilibrium correlation function. One normally does not write the superscript 0 which is usually kept to mean non-interacting system. *From now on, we drop this superscript.*

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[1] We let the density matrix take its initial equilibrium value. This is physically appealing. But we could have as well started from a representation where it is the density matrix that evolves in time and the operators that are constant.

Remark 8 *Translationally invariant case: Since we compute equilibrium averages, the susceptibility $\chi_{BA_i}^R(\mathbf{r}, t; \mathbf{r}', t')$ can depend only on the time difference. In the translationally invariant case, the susceptibility is also a function of only $\mathbf{r} - \mathbf{r}'$ so that Fourier transforming the expression for the linear response (2.52), we obtain from the convolution theorem in this case,*

$$\boxed{\delta \langle B(\mathbf{q}, \omega) \rangle = \chi_{BA_i}^R(\mathbf{q}, \omega) a_i(\mathbf{q}, \omega).} \tag{2.54}$$

Remark 9 *Frequency of the response: The response is at the same frequency as the external field, a feature which does not survive in non-linear response.*

Remark 10 *Onsager reciprocity relations: Given the expression for the response function in terms of a commutator of Hermitian operators, it is clear that the response of the operator B to an external perturbation that couples to A is simply related to the response of A to a perturbation that couples to B, in other words where the operators have reversed roles. These are "Onsager's reciprocity relations".*

Remark 11 *Validity of linear response and heating: Finally, we can ask whether it is really justified to linearize the response. Not always since the external perturbation can be large. But certain arguments suggest that it is basically never correct in practice to linearize the response. Indeed, assume we apply an external electric field E. As long as the energy gained by the action of the field is smaller than $k_B T$, the linearization should be correct. In other words, linear response theory should be valid for a time*

$$t < \frac{k_B T}{eEv}. \tag{2.55}$$

This is unfortunately a ridiculously small time. Taking $v \approx \sqrt{k_B T/m}$ the condition becomes $t < \sqrt{mk_B T}/eE$ with $E = 1V/cm$, $\sqrt{mk_B T}/eE \approx \sqrt{10^{-30} 10^{-23} 10^2}/10^{-19} \approx 10^{-6}s$. Indeed, one finds that unless there is a temperature gradient, or an explicit interaction with a system in equilibrium (such as phonons), the second order term in perturbation theory is secular, i.e. it grows linearly with time. This is nothing more than the phenomenon of Joule heating.[2] We are then forced to conclude that linear response theory applies, only as long as the system is maintained in equilibrium by some means: for example by explicitly including interactions with phonons which are by force taken to be in thermal equilibrium, or by allowing for a thermal gradient in the system that carries heat to the boundaries. In a Boltzmann picture, one can see explicitly that if the second-order term in E is kept small by collisions with a system in thermal equilibrium, then the linear term is basically equal to what we would have obtained by never going to second-order in the first place.[2]

Remark 12 *Reversibility and linear response: Other arguments against linear response theory center on the fact that a correlation function where operators all evolve reversibly cannot describe irreversible processes.[3] We will see explicitly later that it is possible to compute irreversible absorption with this approach. We will also see how irreversibility comes in the infinite-volume limit.*

2.3 General properties of correlation functions

It is useful to know analytic properties that do not depend on the microscopic model considered. This has at least two advantages: a) to check whether approximation schemes satisfy these exact relations b) to formulate phenomenological

relations which are consistent. We will see that approximate calculations cannot satisfy all known exact relations for correlation functions, but it will be obvious that violating certain relations is more harmful than violating others. Many of the general properties which we will discuss in the present context have trivial generalizations for Green's function. Working on these general properties now will make them look more natural later when we introduce the curious Green's function beast!

2.3.1 Notations and definitions

To start with, recall the definition

$$\chi_{BA}^{R}(\mathbf{r}, t; \mathbf{r}', t') = \frac{i}{\hbar} \langle [B(\mathbf{r}, t), A(\mathbf{r}', t')] \rangle \theta(t - t'). \tag{2.56}$$

We have removed the superscript ^{0} which was only used as a crutch in the derivation of linear-response theory to indicate that the operators were evolving with the unperturbed Hamiltonian. Since the unperturbed Hamiltonian in the present context is the full Hamiltonian of the system, including interactions, we will drop the superscript ^{0} from now on. It will be used later in a context where the unperturbed Hamiltonian is that of non-interacting particles.

We define one more correlation function which will, in most cases of physical interest, play the role of the quantity which describes absorption. Welcome χ''

$$\boxed{\chi_{BA}''(\mathbf{r}, t; \mathbf{r}', t') = \frac{1}{2\hbar} \langle [B(\mathbf{r}, t), A(\mathbf{r}', t')] \rangle.} \tag{2.57}$$

The two in the denominator looks strange, but it will allow χ'' to generally be the imaginary part of a response function without extra factors of 2. With this definition, we have

$$\chi_{BA}^{R}(\mathbf{r}, t; \mathbf{r}', t') = 2i\chi_{BA}''(\mathbf{r}, t; \mathbf{r}', t')\theta(t - t'). \tag{2.58}$$

To shorten the notation, we will also use the notation

$$\boxed{\chi_{A_i A_j}^{R}(t - t') = \frac{i}{\hbar} \langle [A_i(t), A_j(t')] \rangle \theta(t - t').} \tag{2.59}$$

In this notation we include in the indices i and j the positions as well as any other label of the operator such as vector or spin component. In this notation, we have not assumed translational invariance. We did however assume time-translation invariance. Since we are working with equilibrium averages above, this is always true.

Exercise 2.3.1 *Check time-translational invariance explicitly by using Heisenberg's representation, the cyclic property of the trace and the fact that the density matrix ($Z^{-1}e^{-\beta H}$ in the canonical ensemble, or $\Xi^{-1}e^{-\beta(H-\mu N)}$ in the grandcanonical) commutes with the time-evolution operator $e^{-iHt/\hbar}$.*

Corresponding to the short-hand notation, we have

$$\boxed{\chi_{A_i A_j}''(t - t') \equiv \frac{1}{2\hbar} \langle [A_i(t), A_j(t')] \rangle.} \tag{2.60}$$

$$\boxed{\chi_{A_i A_j}^{R}(t - t') = 2i\chi_{A_i A_j}''(t - t')\theta(t - t').} \tag{2.61}$$

2.3.2 Symmetry properties of the response functions

The quantity $\chi''_{A_i A_j}(t - t')$ contains all the non-trivial information on the response. Indeed, the causal response is simply obtained by multiplying by a trivial $\theta(t - t')$ function. Certain symmetries of this response function depend on the particular symmetry of the Hamiltonian, others are quite general. Let us consider them in turn.[1]

Properties that depend on the symmetry of the Hamiltonian

Let S be a symmetry of the Hamiltonian. By this we mean that the operator S representing the symmetry commutes with the Hamiltonian

$$[H, S] = 0 \tag{2.62}$$

To be more precise, in the context of statistical mechanics we say that S is a symmetry of the system when it commutes with the density matrix

$$[\rho, S] = 0 \tag{2.63}$$

In other words, $S^{-1}\rho S = \rho$ thus the spectrum of the density matrix is unaffected by the symmetry operation. The operator S is in general unitary or antiunitary as we will see below.

To extract non-trivial consequences of the existence of a symmetry, one first takes advantage of the fact that the trace can be computed in any complete basis set. This means that the thermal average of any operator $\mathcal{O}$ is equal to its thermal average in a basis where the symmetry operation S has been applied to every basis function. Since the symmetry operation commutes with the density matrix by assumption, one can then let the symmetry operations act on the operators instead of on the basis functions. In other words, we have

$$\boxed{\left\langle S^{-1}\mathcal{O}S \right\rangle = \langle \mathcal{O} \rangle} \tag{2.64}$$

It is because S and $\mathcal{O}$ in general do not commute that the above equation leads to non-trivial consequences.

Let us look in turn at the consequences of translational invariance and of invariance under a parity transformation $\mathbf{r}_\alpha \rightarrow -\mathbf{r}_\alpha$. We skip the proofs.

- *Translational invariance:*

$$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} + \mathbf{R}, t; \mathbf{r}' + R, t') \tag{2.65}$$

  so that χ''_{BA} is a function of $\mathbf{r} - \mathbf{r}'$ only. Since we already know that χ''_{BA} is a function only of $t - t'$, in such cases we write

$$\boxed{\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} - \mathbf{r}'; t - t')} \tag{2.66}$$

- *Parity:* Under a parity transformation, operators transform as follows

$$P^{-1}\mathcal{O}(\mathbf{r})P = \varepsilon^P \mathcal{O}(-\mathbf{r}) \tag{2.67}$$

  where $\varepsilon^P = \pm 1$. This number is known as the "signature" under parity transformation. That $\varepsilon^P = \pm 1$ is the only possibility for simple operators like density and momentum follows from the fact that applying the parity operation twice is the same as doing nothing. In other words, $P^2 = 1$.

To be more specific, $\varepsilon_\rho^P = 1$ for density while for the momentum operator, $\varepsilon_p^P = -1$. In general then, this implies that

$$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{r}, t; -\mathbf{r}', t') \qquad (2.68)$$

When we also have translational invariance, the last result means that $\chi''_{BA}(\mathbf{r} - \mathbf{r}'; t - t')$ is even or odd in $\mathbf{r} - \mathbf{r}'$ depending on whether the operators have the same or opposite signatures under parity. Correspondingly, the Fourier transform in the translationally invariant case is odd or even, as can easily be proven by a change of integration variables in the Fourier transform

$$\boxed{\chi''_{BA}(\mathbf{q}; t - t') = \varepsilon_B^P \varepsilon_A^P \chi''_{BA}(-\mathbf{q}; t - t')} \qquad (2.69)$$

- *Time-reversal symmetry in the absence of spin:* From the Schrödinger equation in the absence of spin, one can see that when the Hamiltonian is real, then complex conjugation leads to an equation that evolves the complex conjugate wave function as if $t \to -t$. We thus take time-reversed states as just this operation of complex conjugation. A system in equilibrium obeys time-inversion symmetry, unless an external magnetic field is applied. This means that equilibrium averages evaluated with time-reversed states are equal to equilibrium averages evaluated with the original bases. In fact time-inversion symmetry is a very subtle subject. A very complete discussion may be found in Gottfried [4] and Sakurai [8]. We present an oversimplified discussion. Let us call T_t the operator that time-reverses a state. This is the operation of complex conjugation that we will call K. The first thing to notice it that it is unlike any other operator in quantum mechanics. In particular, the Dirac notation must be used with extreme care. Indeed, for standard operators, say X, we have the associative axiom

$$\langle \alpha | X | \beta \rangle = \langle \alpha | \quad (X | \beta \rangle) = (\langle \alpha | X) \quad | \beta \rangle \qquad (2.70)$$

This is clearly incorrect if X is the complex conjugation operator. Hence, we must absolutely specify if it acts on the right or on the left. Hence, we will write $\underrightarrow{K}$ when we want to take the complex conjugate of a ket, and $\underleftarrow{K}$ to take the complex conjugate of a bra.

Remark 13 *Antiunitary operators: Time reversal is an antiunitary operation. The key property that differentiates an anti-unitary operator from a unitary one is its action on a linear combination*

$$T_t \left(a_1 |\psi_1\rangle + a_2 |\psi_2\rangle \right) = a_1^* T_t |\psi_1\rangle + a_2^* T_t |\psi_2\rangle \qquad (2.71)$$

In general such an operator is called antilinear. Antiunitarity comes in when we restrict ourselves to antilinear operators that preserve the norm. The time reversal operator is such an operator. Under time reversal, an arbitrary matrix element preserves its norm, but not its phase. This is easy to see from the fact that for an arbitrary matrix element $\langle \psi_1 | \underleftarrow{K} \underrightarrow{K} |\psi_2\rangle = \langle \psi_2 | \psi_1 \rangle \neq \langle \psi_1 | \psi_2 \rangle$ the phase changes sign under complex conjugation while the square modulus $\langle \psi_2 | \psi_1 \rangle \langle \psi_1 | \psi_2 \rangle$ is invariant. Gottfried[4] shows that only discrete transformations (not continuous ones) can be described by anti-unitary operators. This reference also discusses the theorem by Wigner that states that if we declare that two descriptions of quantum mechanics are equivalent if $|\langle \psi_2 | \psi_1 \rangle| = |\langle \psi_2' | \psi_1' \rangle|$ (equality of "rays") then both unitary and anti-unitary transformations are allowed.

Remark 14 *The adjoint is not the inverse. Note that $T_t^\dagger T_t = \underleftarrow{K}\,\underrightarrow{K}$, so this last quantity is not the identity because the rightmost complex conjugation operator acts to the right, and the leftmost one to the left. Again, it is not convenient to talk about time-reversal in the usual Dirac notation.*

- Returning to the action of the time reversal operation on a Schrödinger operator, we see that the expectation value of an arbitrary operator between time reversed states is

$$\langle i|\,\underleftarrow{K}\mathcal{O}\underrightarrow{K}\,|j\rangle = \left(\langle i|\,\underleftarrow{K}\right)\left(\underrightarrow{K}\mathcal{O}^*\,|j\rangle\right) = (\langle i|\,\mathcal{O}^*\,|j\rangle)^* = \langle j|\,\mathcal{O}^{\dagger *}\,|i\rangle. \quad (2.72)$$

In the above expression, we used one of the properties of the hermitian product, namely $\langle k\,|l\rangle^* = \langle l\,|k\rangle^*$, as well as the definition of the adjoint of an operator $\mathcal{A}: \langle k|\,\mathcal{A}\,|l\rangle^* = \langle l|\,\mathcal{A}^\dagger\,|k\rangle$. Applying this expression Eq.(2.72) for diagonal expectation values, and recalling that the density matrix is real, we find for equilibrium averages,

$$\left\langle \underleftarrow{K}\mathcal{O}\underrightarrow{K}\right\rangle = \left\langle \mathcal{O}^{\dagger *}\right\rangle = \varepsilon^t\left\langle \mathcal{O}^\dagger\right\rangle \quad (2.73)$$

The last equality defines the signature of the time-reversal operation for operators. One easily finds that $\epsilon^t = +1$ for position while $\epsilon^t = -1$ for velocity or momentum, etc... We can use this last result to find the effect of the time-reversal invariance on general correlation functions. The action of time reversal Eq.(2.73) gives, when A and B are *self-adjoint* operators, and $\underrightarrow{K}H = H\underrightarrow{K}$

$$\begin{aligned}\left\langle \underleftarrow{K}A(t)B\underrightarrow{K}\right\rangle &= \left\langle B^* e^{-iHt/\hbar}A^* e^{iHt/\hbar}\right\rangle \\ &= \epsilon_A^t \epsilon_B^t \left\langle BA(-t)\right\rangle \end{aligned} \quad (2.74)$$

In addition to the signature, the order of operators is changed as well as the sign of time. For $\chi''_{A_i A_j}(t - t')$ this immediately leads to

$$\chi''_{A_i A_j}(t - t') = \epsilon_i^t \epsilon_j^t \chi''_{A_j A_i}(-t' - (-t)) \quad (2.75)$$

and for the corresponding Fourier transform in frequency,

$$\boxed{\chi''_{A_i A_j}(\omega) = \epsilon_i^t \epsilon_j^t \chi''_{A_j A_i}(\omega)}. \quad (2.76)$$

Remark 15 *In the case of an equilibrium average where both the density matrix and the Hamiltonian commute with the time-reversal operation, we have, as in Eq.(2.64),*

$$\left\langle T_t^{-1}\mathcal{O}T_t\right\rangle = \left\langle \mathcal{O}\right\rangle. \quad (2.77)$$

Hence as expected, Eqs.(2.73) and (2.77) together imply that operators that have an odd signature with respect to time reversal symmetry have a vanishing expectation value in equilibrium.

- *Time-reversal symmetry in the presence of spin:* Spin should transform under time reversal like angular momentum $\mathbf{r} \times \mathbf{p}$, in other words it should change sign since $\mathbf{r}$ does not while $\mathbf{p}$ does. Complex conjugation has this property for $\mathbf{r} \times \mathbf{p}$ but not for spin represented by Pauli matrices. We should really wait for the section where we treat fermions to discuss this problem but we can start to address it here. To come out from the problem that complex conjugation does not suffice anymore, it suffices to notice that in

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general the time reversal operator has to be represented by a unitary operator times complex conjugation. The resulting operator is still anti-unitary, as can easily be proven. Let us thus write

$$T_t = \underrightarrow{K}U \tag{2.78}$$

where $\underrightarrow{K}$ is complex conjugation again and U is a unitary operator $U^\dagger U = 1$ in spin space that we need to find. Note that the action on a bra is given by

$$U^\dagger \underleftarrow{K} \tag{2.79}$$

Let us first repeat the steps of calculating expectation values in time-reversed states, as in Eq.(2.72), but for the more general case

$$\langle i| U^\dagger \underleftarrow{K} \mathcal{O} \underrightarrow{K}U |j\rangle = \left(\langle i| U^\dagger \underleftarrow{K}\right)\left(\underrightarrow{K}\mathcal{O}^*U |j\rangle\right) = \left(\langle i| U^\dagger \mathcal{O}^*U |j\rangle\right)^* = \langle j| U^\dagger \mathcal{O}^{\dagger *}U |i\rangle \tag{2.80}$$

Computing the equilibrium trace with $U^\dagger \mathcal{O}^{\dagger *}U$ is thus equivalent to computing the equilibrium trace in time-reversed states but with $\mathcal{O}$. If we take for $\mathcal{O}$ the spin $\boldsymbol{\sigma}$, the net effect of the time-reversal operation should be to change the direction of the spin, in other words, we want

$$U^\dagger \boldsymbol{\sigma}^{\dagger *}U = -\boldsymbol{\sigma} \tag{2.81}$$

The expression for U will depend on the basis states for spin. Using the Pauli matrix basis

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad ; \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad ; \quad \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.82}$$

we have $\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$, and $\sigma_x^* = \sigma_x$, $\sigma_y^* = -\sigma_y$, $\sigma_z^* = \sigma_z$ so that Eq.(2.81) for time reversal gives us the following set of equations for the unitary operator U

$$U^\dagger \sigma_x U = -\sigma_x \tag{2.83}$$

$$U^\dagger \sigma_y U = \sigma_y \tag{2.84}$$

$$U^\dagger \sigma_z U = -\sigma_z \tag{2.85}$$

Given the fundamental properties of Pauli matrices

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 0 \quad \text{for } i \neq j$$

$$\sigma_i^2 = 1 \tag{2.86}$$

$$\sigma_i \sigma_j = i\sigma_k \tag{2.87}$$

where i, j, k are cyclic permutations of x, y, z, the solution to the set of equations for U is

$$U = e^{i\delta}\sigma_y \tag{2.88}$$

where δ is an arbitrary real phase. This is like a π rotation along the y axis so that already we can expect that up will be transformed into down as we were hoping intuitively. In summary, the time reversal operator in the presence of spin multiplies the spin part by $e^{i\delta}\sigma_y$ and takes the complex conjugate.

$$T_t = \underrightarrow{K}e^{i\delta}\sigma_y \tag{2.89}$$

Note the action of this operator on real spinors quantized along the z direction

$$T_t |\uparrow\rangle = -ie^{-i\delta} |\downarrow\rangle \tag{2.90}$$

$$T_t \left| \downarrow \right\rangle = ie^{-i\delta} \left| \uparrow \right\rangle \tag{2.91}$$

The time reversal operator thus transforms up into down and vice versa but with a phase. Even if we can choose $e^{-i\delta} = i$ to make the phase real, the prefactor cannot be $+1$ for both of the above equations. In particular, note that $T_t T_t \left| \uparrow \right\rangle = - \left| \uparrow \right\rangle$, another strange property of spinors. The application of two time reversal operations on spinors is like a 2π rotation around y so that it changes the phase of the spinor. It can be proven that this result is independent of the choice of quantization axis, as we can expect.[4] As far as the main topic of the present section is concerned, observables such as angular momentum will have a simple signature under time reversal (they are always two spinors that come in for each observable A_i) so that the results of the previous section are basically unmodified.

When $\chi''_{A_i A_j}(\omega)$ is real, the properties of being a commutator (2.93) and of Hermiticity (2.95) allow us to further show that $\chi''_{A_i A_i}(\omega)$ is also an odd function of frequency, an important result that we show in the following section.

Properties that follow from the definition.

Let us thus write down the general symmetry properties of $\chi''_{A_i A_j}(t - t')$ that simply follow from its definition (2.60).

- *Commutator:* Since it is a commutator, we have

$$\chi''_{A_i A_j}(t - t') = -\chi''_{A_j A_i}(t' - t) \tag{2.92}$$

  which in frequency space reads,

$$\boxed{\chi''_{A_i A_j}(\omega) = -\chi''_{A_j A_i}(-\omega)}. \tag{2.93}$$

- *Hermiticity:* Taking the observables as Hermitian, as is usually the case, one can use the cyclic property of the trace and the Hermiticity of the density matrix to show that

$$\chi''_{A_i A_j}(t - t') = \left[\chi''_{A_j A_i}(t' - t) \right]^* . \tag{2.94}$$

(Proof for Hermitian operators: $\langle [A_i, A_j] \rangle^* = Tr \{\rho A_i A_j - \rho A_j A_i\}^*$

$= Tr \{A_j A_i \rho - A_i A_j \rho\} = Tr \{\rho [A_j, A_i]\}$ with ρ the density matrix.)

In Fourier space, this becomes,

$$\boxed{\chi''_{A_i A_j}(\omega) = \left[\chi''_{A_j A_i}(\omega) \right]^*}. \tag{2.95}$$

Remark 16 *Non-hermitian operators: It is important to note that the operators A_i may be non-Hermitian, as is the case for superconductivity. In such cases, one should remember that the above property may not be satisfied.*

Remark 17 *Most useful property: The most important consequence of this section that we will often use is that correlation functions such as $\chi''_{\rho_\mathbf{q} \rho_{-\mathbf{q}}}(\omega)$ are odd in frequency and real*

$$\boxed{\chi''_{\rho_\mathbf{q} \rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_\mathbf{q} \rho_{-\mathbf{q}}}(-\omega) = \left[\chi''_{\rho_\mathbf{q} \rho_{-\mathbf{q}}}(\omega) \right]^*} \tag{2.96}$$

To prove this, we first use Hermiticity Eq.(2.95) in the form

$$\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* \tag{2.97}$$

to show that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ is real

$$\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = \int d^3\mathbf{r} \int d^3\mathbf{r}' e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) \tag{2.98}$$

$$= \left[\int d^3\mathbf{r} \int d^3\mathbf{r}' e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^* \tag{2.99}$$

$$= \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^* \tag{2.100}$$

The commutator property Eq.(2.93), $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega)$ and symmetry under parity transformation Eq.(2.69), $\chi''_{\rho_{-\mathbf{q}}\rho_{\mathbf{q}}}(-\omega) = \chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$ then suffice to show that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ is also odd in frequency $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$. Instead of parity, one could have invoked time-reversal symmetry Eq.(2.76) and the commutator property Eq.(2.93) to show that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)$ is odd since then $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega) = -\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(-\omega)$ immediately implies that $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$.

2.3.3 Kramers-Kronig relations and causality

These Kramers-Kronig relations are by far the best known and most useful relations. They relate real and imaginary parts of response functions and they come simply from causality. Causality is insured by the presence of the θ function in the expression for the response functions Eq.(2.61). Causality simply states that the response to an applied field at time t' occurs only at time t later. This is satisfied in general in our formalism, as can be seen by looking back at the formula for the linear response Eq.(2.52). Kramers-Kronig relations are the same causality statement as above, seen from the perspective of Fourier transforms. To be more specific, in this section we will derive the following results:

$$\boxed{\text{Re}\left[\chi^R_{A_i A_j}(\omega)\right] = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\text{Im}\left[\chi^R_{A_i A_j}(\omega')\right]}{\omega'-\omega}} \tag{2.101}$$

$$\boxed{\text{Im}\left[\chi^R_{A_i A_j}(\omega)\right] = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\text{Re}\left[\chi^R_{A_i A_j}(\omega')\right]}{\omega'-\omega}.} \tag{2.102}$$

They come from analytic properties of the response functions in the complex frequency plane. We give two derivations.

The straightforward manner:

Let us first derive the relations the easy way. Suppose that we know the Fourier transform in frequency $\chi^R_{A_i A_j}(\omega)$ of the response function. We call it the retarded function because the response comes after the perturbation. It is causal. One way to make sure that its real time version $\chi^R_{A_i A_j}(t-t')$ contains $\theta(t-t')$ is to have $\chi^R_{A_i A_j}(\omega)$ analytic in the upper half-plane. To see that analyticity in the upper half-plane is a sufficient condition to have $\theta(t-t')$, consider

$$\chi^R_{A_i A_j}(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')}\chi^R_{A_i A_j}(\omega). \tag{2.103}$$

If $t - t'$ is negative, then it is possible to close the contour in the upper half plane since the exponential will decrease at positive imaginary frequencies. Since $\chi^R_{A_i A_j}(\omega)$ is analytic in that half-plane, the result will be zero, which is just another way to say that $\chi^R_{A_i A_j}(t - t')$ is proportional to $\theta(t - t')$, as we had planned to show. In the next subsection, we will show that analyticity in the upper half plane is also a necessary condition to have $\theta(t - t')$.

Assuming that $\chi^R_{A_i A_j}(\omega)$ is analytic in the upper half plane, it is then easy to derive the Kramers-Kronig relations. It now suffices to use

$$\int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\eta} \chi^R_{A_i A_j}(\omega') = 2i\chi^R_{A_i A_j}(\omega + i\eta) \tag{2.104}$$

which is easy to prove by applying the residue theorem on a contour closed in the upper half plane where $\chi^R_{A_i A_j}(\omega)$ is analytic. This also assumes that $\chi^R_{A_i A_j}(\omega')$ falls off at least like a small power of $1/\omega'$ so that there is no contribution from the part at ∞. We then need the following identity,

$$\lim_{\eta \to 0} \frac{1}{\omega \mp i\eta} = \lim_{\eta \to 0} \frac{\omega \pm i\eta}{\omega^2 + \eta^2} = \lim_{\eta \to 0} \left[\frac{\omega}{\omega^2 + \eta^2} \pm \frac{i\eta}{\omega^2 + \eta^2} \right] = \mathcal{P}\frac{1}{\omega} \pm i\pi\delta(\omega) \tag{2.105}$$

where δ is Dirac's delta function and $\mathcal{P}$ means principal part integral. — Suppose the factor $1/(\omega + i\eta)$ on the left is in an integral that can be done by contour integration. Then, knowing the definition of the delta function, this can be used as the definition of principal part.— Using this identity and setting equal the real parts of our contour integral (2.104) we obtain, upon taking the $\lim \eta \to 0$,

$$\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\left[\chi^R_{A_i A_j}(\omega')\right]}{\omega' - \omega} - \mathrm{Im}\left[\chi^R_{A_i A_j}(\omega)\right] = -2\,\mathrm{Im}\left[\chi^R_{A_i A_j}(\omega)\right] \tag{2.106}$$

while from the imaginary part,

$$\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\left[\chi^R_{A_i A_j}(\omega')\right]}{\omega' - \omega} + \mathrm{Re}\left[\chi^R_{A_i A_j}(\omega)\right] = 2\,\mathrm{Re}\left[\chi^R_{A_i A_j}(\omega)\right]. \tag{2.107}$$

This is precisely what we mean by the Kramers-Kronig relations, namely we recover the results Eqs.(2.101)(2.102) at the beginning of this section. From the proof just given, Kramers-Kronig relations will apply if

- $\chi^R_{A_i A_j}(\omega)$ is analytic, as a function of complex frequency, in the upper half-plane.

- $\chi^R_{A_i A_j}(\omega)$ falls off at least as a small power of ω at infinity.

Spectral representation and alternate derivation.

It is instructive to perform a derivation which starts from what we found earlier. We will gain as a bonus an explicit expression for real and imaginary parts in terms of correlation functions, as well as a derivation of the analyticity properties from scratch. In fact this will also complete the proof that analyticity in the upper half-plane is both necessary and sufficient to have causality.

Using the convolution theorem, we would write for the frequency-space version of the response functions, (2.61)

$$\chi^R_{A_i A_j}(\omega) = 2i \int \frac{d\omega'}{2\pi} \chi''_{A_i A_j}(\omega')\theta(\omega - \omega'). \tag{2.108}$$

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This looks nice, but it does not really mean anything yet because we encounter a serious problem when we try to evaluate the Fourier transform of the θ function. Indeed,

$$\int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) = \frac{e^{i\omega t}}{i\omega}|_0^\infty \tag{2.109}$$

and we have no idea what $e^{i\omega\infty}$ means. To remedy this, we have to return to the expression for the linear response (2.52). Assuming that the external field a_i is turned-on adiabatically from $t = -\infty$, we multiply whatever we had before by $e^{\eta t'}$, taking the limit of vanishing η at the end of the calculation. We also adiabatically turn off the *response* at $t \to \infty$ by using a factor $e^{-\eta t}$. The equation for the response in time (2.61) is then simply multiplied by $e^{\eta(t'-t)}$, so that it still depends only on the time difference. Furthermore, when we take its Fourier transform, $\int_{-\infty}^{\infty} d(t - t') e^{i\omega(t-t')}$, everything proceeds as before, except that we can use the extra convergence factor $e^{-\eta(t-t')}$, to make sense out of the Fourier transform of the Heaviside theta function. To be more specific, the equation for the response (2.61) now reads,

$$\chi_{A_i A_j}^R (t - t') e^{-\eta(t-t')} = 2i\chi_{A_i A_j}''(t - t')\theta(t - t')e^{-\eta(t-t')} \tag{2.110}$$

so that in the calculation of the response (2.108) we have,

$$\int_{-\infty}^{\infty} d(t - t') e^{i(\omega+i\eta-\omega')(t-t')}\theta(t - t') = \frac{e^{i(\omega+i\eta-\omega')(t-t')}}{i(\omega + i\eta - \omega')}|_0^\infty = \frac{1}{i(\omega' - \omega - i\eta)}. \tag{2.111}$$

Everything behaves as if we had computed the Fourier transform for $\omega + i\eta$ instead of ω,

$$\chi_{A_i A_j}^R (\omega + i\eta) = 2i \int \frac{d\omega'}{2\pi} \chi_{A_i A_j}''(\omega')\theta(\omega + i\eta - \omega') \tag{2.112}$$

$$= \int \frac{d\omega'}{\pi} \frac{\chi_{A_i A_j}''(\omega')}{\omega' - (\omega + i\eta)}. \tag{2.113}$$

This function is called the "retarded response" to distinguish it from what we would have obtained with $\theta(t' - t)$ instead of $\theta(t - t')$. The retarded response is causal, in other words, the response occurs only after the perturbation. In the anti-causal case ("advanced response") the response all occurs *before* the perturbation is applied. In the latter case, the convergence factor is $e^{-\eta(t'-t)}$ instead of $e^{\eta(t'-t)}$. Introducing a new function

$$\boxed{\chi_{A_i A_j}(z) = \int \frac{d\omega'}{\pi} \frac{\chi_{A_i A_j}''(\omega')}{\omega' - z}} \tag{2.114}$$

we can write for the retarded response,

$$\boxed{\chi_{A_i A_j}^R (\omega) = \lim_{\eta \to 0} \chi_{A_i A_j}(z)|_{z=\omega+i\eta}} \tag{2.115}$$

and for the advanced one,

$$\boxed{\chi_{A_i A_j}^A (\omega) = \lim_{\eta \to 0} \chi_{A_i A_j}(z)|_{z=\omega-i\eta}.} \tag{2.116}$$

Using the above results, it is easy to see that $\chi_{A_i A_j}^R (\omega)$ is analytic in the upper half plane, while $\chi_{A_i A_j}^A (\omega)$ is analytic in the lower-half plane. One can even explicitly see from the equation (2.113) for the function which is analytic in the upper-half plane $\chi_{A_i A_j}^R (\omega)$ that the poles or the integrand in the lower-half frequency plane are just below the real axis, a distance η along the imaginary direction. The residue at a given pole will depend on the value of $\chi_{A_i A_j}''$ at the corresponding value of the real coordinate of the pole.

Remark 18 *If $\chi''_{A_i A_j}(\omega')$ is given by a sum of delta function, then $\chi_{A_i A_j}(z)$ has a series of poles just below the real axis. This is what occurs with the so-called Lehman representation that we will discuss later. On the other hand, if $\chi''_{A_i A_j}(\omega')$ is a continuous function, as occurs in an infinite system, then the poles of $\chi_{A_i A_j}(z)$ are below the real axis, but not necessarily close to it. The passage from a series of poles to a continuous function is what introduces irreversibility in many-body systems.*

Definition 4 *Equations such as (2.114) are called spectral representations.*

Remark 19 *Why spectral representation: The reason for this name is that, as we discuss in the next section below, $\chi''_{A_i A_j}(\omega')$ contains information on dissipation or, alternatively, on the spectrum of excitations. Hence, in that kind of equations, the response is expressed in terms of the spectrum of excitations. We will also have spectral representations for Green's functions.*

$\chi_{A_i A_j}(z)$ is a function which is equal to $\chi^R_{A_i A_j}(\omega)$ for z infinitesimally above the real axis, and to $\chi^A_{A_i A_j}(\omega)$ for z infinitesimally below the real axis. On the real axis of the complex z plane $\chi_{A_i A_j}(z)$ has a cut whenever $\chi''_{A_i A_j}(\omega) \neq 0$ since

$$\left[\chi_{A_i A_j}(\omega + i\eta) - \chi_{A_i A_j}(\omega - i\eta) \right] = 2i\chi''_{A_i A_j}(\omega). \tag{2.117}$$

So much for taking the Fourier transform of a response which is so simple looking in its ordinary time version Eq.(2.61). Time-reversal invariance (2.76) and Hermiticity in Eq.(2.95) imply, for two operators with the same signature under time-reversal, that $\chi''_{A_i A_j}(\omega')$ is a real function. Hence, from the mathematical identity for principal part Eq.(2.105) and from the spectral representation (2.114) we have, *for two hermitian operators A_i, A_j with the same signature under time reversal,* that

$$\boxed{\mathrm{Im}\left[\chi^R_{A_i A_j}(\omega) \right] = \chi''_{A_i A_j}(\omega)} \tag{2.118}$$

so that from the spectral representation we recover the first of the Kramers-Krönig relation (2.101). The other one can be derived following the same route as in the simpler derivation, namely apply $\int \frac{d\omega}{\pi} \frac{1}{\omega - \omega' + i\eta}$ on both sides of the spectral representation. *For two hermitian operators A_i, A_j with opposite signatures under time reversal* Eqs.(2.76) and (2.95) imply that $\chi''_{A_i A_j}(\omega')$ is purely imaginary. In this case,

$$\boxed{\mathrm{Re}\left[\chi^R_{A_i A_j}(\omega) \right] = i\chi''_{A_i A_j}(\omega)}. \tag{2.119}$$

Remark 20 *Kramers-Kronig and time reversal: The Kramers Krönig relations do not depend on these subtleties of signatures under time-reversal. However the relation between real and imaginary parts of the response and commutator Eq.(2.118) does. If we can compute either the real or imaginary part of the response, the Kramers Krönig relations give us the part we do not know. In any case, everything about the system is in $\chi''_{A_i A_j}(\omega)$.*

2.3.4 Positivity of $\omega\chi''(\omega)$ and dissipation

Without proof, we state that positivity of dissipation implies that

$$\boxed{\chi''_{A_i A_i}(\omega)\omega > 0.} \tag{2.120}$$

We have seen that for Hermitian operators with the same signature under time reversal, $\chi''_{A_iA_i}(\omega)$ is a real and odd function of frequency so the above equation is satisfied. The positive definiteness of $\chi''_{A_iA_j}(\omega)\omega$ by itself however does not suffice to prove that $\chi''_{A_iA_i}(\omega)$ is an odd function of frequency.

One can check explicitely that $\chi''_{A_iA_i}(\omega)$ contains spectral information about excited states by doing backwards the steps that lead us from Fermi's golden rule to correlation functions.

2.3.5 Fluctuation-dissipation theorem

This very useful theorem relates linear response to equilibrium fluctuations measured in scattering experiments. It takes the form,

$$\boxed{S_{A_iA_j}(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega) = 2\hbar(1+n_B(\omega))\chi''_{A_iA_j}(\omega)} \qquad (2.121)$$

where $n_B(\omega) = 1/\left(e^{\beta\hbar\omega}-1\right)$ is the Bose factor while the "structure factor" or correlation function is defined by,

$$S_{A_iA_j}(t) \equiv \langle A_i(t)A_j\rangle - \langle A_i\rangle\langle A_j\rangle = \langle(A_i(t)-\langle A_i\rangle)(A_j(0)-\langle A_j\rangle)\rangle \qquad (2.122)$$

$$\equiv \langle\delta A_i(t)\delta A_j\rangle. \qquad (2.123)$$

We have already encountered the charge structure factor in the context of inelastic neutron scattering. Clearly, the left-hand side of the fluctuation-dissipation theorem Eq.(2.121) is a correlation function for dissipation while the right-hand side contains the dissipation function χ'' just discussed. This is a key theorem of statistical physics.

To prove the theorem, it suffices to trivially relate the definitions,

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\langle[A_i(t),A_j]\rangle = \frac{1}{2\hbar}\langle[\delta A_i(t),\delta A_j]\rangle = \frac{1}{2\hbar}\left(S_{A_iA_j}(t)-S_{A_jA_i}(-t)\right) \qquad (2.124)$$

then to use the key identity,

$$\boxed{S_{A_jA_i}(-t) = S_{A_iA_j}(t-i\hbar\beta)}. \qquad (2.125)$$

This kind of periodicity of equilibrium correlation functions will be used over and over in the context of Green's functions. It will allow to define Fourier expansions in terms of so-called Matsubara frequencies. The proof of the identity simply uses the definition of the time evolution operator and the cyclic property of the trace. More specifically, using the cyclic property of the trace, time-translation invariance follows, and

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}\delta A_j(-t)\delta A_i\right] = Z^{-1}Tr\left[e^{-\beta H}\delta A_j\delta A_i(t)\right] \qquad (2.126)$$

To reverse the order of δA_i and δA_j, it suffices to use the cyclic property, so that

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[\delta A_i(t)e^{-\beta H}\delta A_j\right]. \qquad (2.127)$$

Simple manipulations and Heisenberg's representation for the time-evolution of the operators gives,

$$S_{A_jA_i}(-t) = Z^{-1}Tr\left[e^{-\beta H}e^{\beta H}\delta A_i(t)e^{-\beta H}\delta A_j\right] \qquad (2.128)$$

$$= Z^{-1} Tr \left[e^{-\beta H} \delta A_i(t - i\hbar\beta) \delta A_j \right] = S_{A_i A_j}(t - i\hbar\beta). \qquad (2.129)$$

This is precisely what we wanted to prove. The rest is an exercise in Fourier transforms,

$$\int dt e^{i\omega t} S_{A_i A_j}(t - i\hbar\beta) = \int dt e^{i\omega(t + i\hbar\beta)} S_{A_i A_j}(t) = e^{-\beta\hbar\omega} S_{A_i A_j}(\omega). \qquad (2.130)$$

To prove the last result, we had to move the integration contour from t to $t + i\hbar\beta$, in other words in the imaginary time direction. Because of the convergence factor $e^{-\beta H}$ in the traces, expectations of any number of operators of the type $e^{iHt} A e^{-iHt}$ are analytic in the imaginary time direction for $-i\hbar\beta < t < i\hbar\beta$, hence it is permissible to displace the integration contour as we did. Fourier transforming the relation between $\chi''_{A_i A_j}(t)$ and susceptibility Eq.(2.124), one then recovers the fluctuation-dissipation theorem (2.121).

A few remarks before concluding.

Remark 21 *Alternate derivation: Formally, the Fourier transform gives the same result as what we found above if we use the exponential representation of the Taylor series,*

$$S_{A_i A_j}(t - i\hbar\beta) = e^{-i\hbar\beta \frac{\partial}{\partial t}} S_{A_i A_j}(t).$$

Remark 22 *Relation to detailed balance: The Fourier-space version of the periodicity condition (2.125) is a statement of detailed balance:*

$$\boxed{S_{A_j A_i}(-\omega) = e^{-\beta\hbar\omega} S_{A_i A_j}(\omega)}. \qquad (2.131)$$

Indeed, in one case the energy $\hbar\omega$ is absorbed in the process, while in the other case it has the opposite sign (is emitted). This is one way of seeing the basic physical reason for the existence of the fluctuation-dissipation theorem: Even though the response apparently had two different orders for the operators, the order of the operators in thermal equilibrium can be reversed using the cyclic property of the trace..

Remark 23 *Physical explanation of fluctuation-dissipation theorem: Physically, the fluctuation-dissipation theorem is a statement that the return to equilibrium is governed by the same laws, whether the perturbation was created by an external field or by a spontaneous fluctuation.*

2.3.6   Sum rules

All the many-body Physics of the response or scattering experiments is in the calculation of unequal-time commutators. These commutators in general involve the time evolution of the systems and thus they are non-trivial to evaluate. However, equal-time commutators are easy to evaluate in general using the usual commutation relations. Equal-time corresponds to integral over frequency as seen from Fourier space. Hence the name sum rules. We will not in general be able to satisfy all possible sum-rules since this would mean basically an exact solution to the problem, or computing infinite-order high-frequency expansion. In brief, sum-rules are useful to

- Relate different experiments to each other.

- Establish high frequency limits of correlation functions.

- Provide constraints on phenomenological parameters or on approximate theories.

Thermodynamic sum-rules.

Suppose we compute the linear response to a time-independent perturbation. For example, compute the response of the magnetization to a time-independent magnetic field. This should give us the susceptibility. Naturally, we have to leave the adiabatic switching-on, i.e. the infinitesimal η. In general then,

$$\delta \langle A_i(\omega = 0)\rangle = \chi^R_{A_i A_j}(\omega = 0)a_j(\omega = 0). \tag{2.132}$$

Returning to the notation where $\mathbf{q}$ is explicitly written,

$$\delta \langle A_i(\mathbf{q},\omega = 0)\rangle = \chi^R_{A_i A_j}(\mathbf{q},\omega = 0)a_j(\mathbf{q}, \omega = 0). \tag{2.133}$$

Using the spectral representation (2.114) and the usual relation between $i\eta$ and principal parts, Eq.(2.105), we also have,

$$\chi^R_{A_i A_j}(\mathbf{q},\omega = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q},\omega)}{\omega - i\eta} = \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q},\omega)}{\omega}. \tag{2.134}$$

There is no contribution from the imaginary part on the grounds that there can be no dissipation zero-frequency dissipation in a stable system. In fact, as long as the thermodynamic derivatives involve operators that have the same symmetry under time reversal, then $\chi''_{A_i A_j}(\mathbf{q},\omega)$ is odd, as proven at the end of the section on symmetry properties, so that $\chi''_{A_i A_j}(\mathbf{q},\omega = 0) = 0$. Note that in practice, the principal part in the above equation is not necessary since $\chi''_{A_i A_j}(\mathbf{q},\omega)$ usually vanishes linearly in ω for small ω. To be completly general however, it is preferable to keep the principal part.

Recalling that the thermodynamic derivatives are in general for uniform ($\mathbf{q} = 0$) applied probes, the above formula become,

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{A_i A_j}(\mathbf{q},\omega = 0) = \frac{\partial A_i}{\partial a_j} \equiv \chi_{A_i A_j}. \tag{2.135}$$

$$\boxed{\chi_{A_i A_j} = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q},\omega)}{\omega}} \tag{2.136}$$

This is called a thermodynamic sum-rule. As an example, consider the density n response. It obeys the so-called compressibility sum rule,

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{nn}(\mathbf{q},\omega = 0) = \lim_{\mathbf{q}\to\mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} = \left(\frac{\partial n}{\partial \mu}\right)_{T,V}. \tag{2.137a}$$

As usual, a few remarks are in order:

Remark 24 *Order of limits: It is extremely important to note that for thermodynamic sume rules, the $\omega \to 0$ limit is taken first, before the $\mathbf{q} \to 0$ limit. The other limit describes transport properties as we shall see. Another important question is that of the principal part integral. As follows from a problem set, in the long wave length limit we have $\chi''_{nn}(\mathbf{q},\omega) = \frac{2Dq^2\omega}{\omega^2+(Dq^2)^2}\chi_{nn}$ where D is the diffusion constant. One can check explicitly with that form that at any finite q, it does not matter whether we take or not the principal part integral. We did not take it in Eq.(2.137a). If we take the limit $\mathbf{q} \to \mathbf{0}$ before doing the integral however, $\lim_{\mathbf{q}\to\mathbf{0}} \chi''_{nn}(\mathbf{q},\omega)$ takes the form $\omega\delta(\omega)$ so it is important NOT to take the principal part integral to get the correct result (in other words, under the integral sign the $\eta \to 0$ limit must be taken before the $\mathbf{q} \to \mathbf{0}$ limit). We also see this as follows. If we return to the original form $\lim_{\eta\to0} 1/(\omega - i\eta) = \lim_{\eta\to0} \omega/(\omega^2 + \eta^2) + i\eta/(\omega^2 + \eta^2)$, and then do the integral of the first term (real*

part), we can check that we have to take the $\eta \to 0$ limit under the integral sign before the $\mathbf{q} \to \mathbf{0}$ limit to recover the result obtained by doing the integral at finite $\mathbf{q}$ and then taking the $\mathbf{q} \to \mathbf{0}$ limit (the latter is unambiguous and does not depend on the presence of the principal part in the integral). Physically, this means that the adiabatic turning-on time must be longer than the diffusion time to allow the conserved quantity to relax. This is summarized by the following set of equations

$$\lim_{\mathbf{q} \to \mathbf{0}} \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \quad = \quad \lim_{\mathbf{q} \to \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \tag{2.137b}$$

$$= \quad \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q} \to \mathbf{0}} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \tag{2.137c}$$

$$\neq \quad \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q} \to \mathbf{0}} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \tag{2.137d}$$

Remark 25 *Thermodynamic sum-rule and moments: Thermodynamic sum-rules are in a sense the inverse first moment over frequency of $\chi''_{A_i A_j}(\mathbf{q},\omega)$ (the latter being analogous to the weight). Other sum-rules are over positive moments, as we now demonstrate.*

Alternate derivation: Here is another way to derive the thermodynamic sum rules. First note that thermodynamic variables involve conserved quantities, namely quantities that commute with the Hamiltonian. Take for example N, the total number of particles. Since N commutes with the Hamiltonian, in the grand-canonical ensemble we have the classical result

$$\langle NN \rangle - \langle N \rangle^2 = \frac{1}{\beta} \left(\frac{\partial n}{\partial \mu} \right)_{T,V}$$

By definition,

$$\langle NN \rangle - \langle N \rangle^2 = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{NN}(\omega) \tag{2.137e}$$

Using the general fluctuation-dissipation theorem, we now relate this quantity to $\chi''_{NN}(\omega)$ as follows. Because $n_{\mathbf{q}}$ for $\mathbf{q} = \mathbf{0}$ is simply the total number of particles N and hence is conserved, $\langle n_{\mathbf{q}=\mathbf{0}}(t) n_{\mathbf{q}=\mathbf{0}} \rangle$ is time independent. In frequency space then, this correlation function is a delta function in frequency. For such a conserved quantity, the fluctuation-dissipation theorem Eq.(2.121) then becomes

$$S_{NN}(\omega) = \lim_{\omega \to 0} \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \chi''_{NN}(\omega) = \frac{2}{\beta\omega} \chi''_{NN}(\omega) \tag{2.137f}$$

from which we obtain what is basically the thermodynamic sum-rule Eq.(2.137a)

$$\langle NN \rangle - \langle N \rangle^2 \quad = \quad \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{NN}(\omega) \tag{2.137g}$$

$$= \quad \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{NN}(\omega)}{\beta\omega} = \frac{1}{\beta} \left(\frac{\partial n}{\partial \mu} \right)_{T,V} \tag{2.137h}$$

This is then the classical form of the fluctuation-dissipation theorem. In this form, the density fluctuations are related to the response $(\partial n / \partial \mu)_{T,V}$ (itself related to the compressibility).

Moments, sum rules, and high-frequency expansions.

Odd derivatives of $\chi''_{A_i A_j}$ at equal-time are easy to compute and provide us with moments:

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \chi''_{A_i A_j}(\omega) = \left(i \frac{\partial}{\partial t} \right)^n \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} 2\chi''_{A_i A_j}(\omega) \right]_{t=0} \tag{2.137i}$$

$$= \frac{1}{\hbar} \left\langle \left[\left(i\frac{\partial}{\partial t} \right)^n A_i(t), A_j(0) \right] \right\rangle_{t=0} = \frac{1}{\hbar} \left\langle \left[\left[\left[A_i(t), \frac{H}{\hbar} \right], \frac{H}{\hbar} \right] \dots, A_j(0) \right] \right\rangle_{t=0}$$

(2.137j)

which may all easily be computed through n equal-time commutations with the Hamiltonian.

Suppose the spectrum of excitations is bounded, as usually happens when the input momentum $\mathbf{q}$ is finite. Then, $\chi''_{A_i A_j}(\omega') = 0$ for $\omega' > D$ where D is some large frequency. Then, for $\omega > D$, we can expand the denominator since the condition $\omega'/\omega \ll 1$ will always be satisfied. This gives us a high-frequency expansion,

$$\boxed{\chi^R_{A_i A_j}(\mathbf{q},\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_i A_j}(\mathbf{q},\omega')}{\omega' - \omega - i\eta}}$$

(2.137k)

$$\boxed{\approx \sum_{n=1}^{\infty} \frac{-1}{\omega^{2n}} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} (\omega')^{2n-1} \chi''_{A_i A_j}(\mathbf{q},\omega')}$$

(2.137l)

where we have explicitly taken into account the fact that only odd moments of $\chi''_{A_i A_j}$ do not vanish because it is an odd function. Clearly, in the $\omega \to \infty$ limit, the susceptibilities in general scale as $1/\omega^2$, a property we will use later in the context of analytic continuations.

The f sum-rule as an example.

When the potential-energy part of the Hamiltonian commutes with the density operator, while the kinetic-energy part is that of free electrons (not true for tight-binding electrons) we find that

$$\boxed{\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q}, \omega) = \frac{n\mathbf{q}^2}{m}.}$$

(2.137m)

This is the f sum-rule. It is valid for an arbitrary value of the wave vector $\mathbf{q}$. It is a direct consequence of the commutation-relation between momentum and position, and has been first discussed in the context of electronic transitions in atoms. The proof is as follows. We first use the above results for moments

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q}, \omega) = \frac{i}{\hbar \mathcal{V}} \left\langle \left[\frac{\partial n_\mathbf{q}(t)}{\partial t}, n_{-\mathbf{q}}(t) \right] \right\rangle$$

(2.137n)

$$= -\frac{1}{\hbar^2 \mathcal{V}} \left\langle [[H, n_\mathbf{q}(t)], n_{-\mathbf{q}}(t)] \right\rangle$$

(2.137o)

In the first equality, we have also used translational invariance to write,

$$\int d(\mathbf{r} - \mathbf{r}') e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} f(\mathbf{r} - \mathbf{r}') = \frac{1}{\mathcal{V}} \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \int d\mathbf{r}' e^{-i\mathbf{q}\cdot\mathbf{r}'} f(\mathbf{r} - \mathbf{r}')$$

(2.137p)

where $\mathcal{V}$ is the integration volume. The computation of the equal-time commutator is self-explanatory,

$$n_\mathbf{q} = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \sum_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha) = \sum_\alpha e^{-i\mathbf{q}\cdot\mathbf{r}_\alpha}$$

(2.137q)

$$[p^x_\beta, n_\mathbf{q}] = \frac{\hbar}{i} \left[\frac{\partial}{\partial x_\beta}, \sum_\alpha e^{-i\mathbf{q}\cdot\mathbf{r}_\alpha} \right] = -\hbar q^x e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}.$$

(2.137r)

Assuming that the interactions commute with the density operator, and using $[\mathbf{p} \cdot \mathbf{p}, n] = \mathbf{p}[\mathbf{p}, n] + [\mathbf{p}, n]\mathbf{p}$ we have

$$[H, n_\mathbf{q}(t)] = \sum_\beta \left[\frac{p^2_\beta}{2m}, n_\mathbf{q} \right] = \frac{1}{2m} \sum_\beta \left(\mathbf{p}_\beta \cdot (-\hbar \mathbf{q} e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}) + (-\hbar \mathbf{q} e^{-i\mathbf{q}\cdot\mathbf{r}_\beta}) \cdot \mathbf{p}_\beta \right)$$

(2.137s)

$$[[H, n_{\mathbf{q}}(t)], n_{-\mathbf{q}}(t)] = -\frac{1}{m} \sum_{\beta=1}^{N} \hbar^2 \mathbf{q}^2 e^{-i\mathbf{q} \cdot \mathbf{r}_\beta} e^{i\mathbf{q} \cdot \mathbf{r}_\beta} = -\frac{\hbar^2 \mathbf{q}^2 N}{m} \qquad (2.137\text{t})$$

which proves the result (2.137m) when substituted in the expression in terms of commutator (2.137o) with $n \equiv N/\mathcal{V}$. The result of the commutators is a number not an operator, so the thermodynamic average is trivial in this case! (Things will be different with tight-binding models.)

3. GREEN FUNCTIONS

We are now ready to start working with the real many-body problem. This chapter will be rather formal but we will make the link with the previous chapter and also we will try to do applications as soon as possible in the following chapter.

The single-particle basis state is a complete basis that is used most often. Note however that a simple wave-function such as

$$\psi(x, y) = (x - y) N e^{-|x-y|/a} \tag{3.1}$$

for two electrons in one dimension, with N and a constants, is a perfectly acceptable antisymmetric wave function. To expand it in a single-particle basis state however requires a sum over many (in general an infinite number of) anti-symmetrized one-particle states.

The plan then is as follows. We will then motivate the definition of the Green's function in the many-body context by analogy with what we just saw. Then, we return to perturbation theory to show that it is most natural to work in imaginary time. This leads us to the Matsubara Green's function. We show that if we know this Green's function, we also happen to know the retarded one, as well as all the one-body quantities of physical interest. We will once more spend some time on the interpretation of the spectral weight, develop some formulas for working with the Fourier series representation of the imaginary time functions (Matsubara frequencies). This should put us in a good position to start doing perturbation theory, which is all based on Wick's theorem. Hence, we will spend some time proving this theorem as well as the very general linked-cluster theorem that is very useful in practice.

3.0.7 Second quantized operators in the Heisenberg picture

In a previous chapter, we showed how to translate one- and two-body operators in the Schrödinger picture into the language of second quantization. The Heisenberg picture is defined as usual. In this section, we derive a few useful identities and study the case of quadratic Hamiltonians as an example.

In the Heisenberg picture

$$\boxed{c_{\mathbf{k}}(t) = e^{i\widehat{H}t} c_{\mathbf{k}} e^{-i\widehat{H}t} \quad ; \quad c_{\mathbf{k}}^{\dagger}(t) = e^{i\widehat{H}t} c_{\mathbf{k}}^{\dagger} e^{-i\widehat{H}t}} \tag{3.2}$$

It is easy to compute the time evolution in the case where the Hamiltonian is quadratic in creation and annihilation operators. Take for example

$$\widehat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \tag{3.3}$$

The time evolution may be found from the Heisenberg equation of motion, which follows from differentiating the definition of the Heisenberg operators

$$i\frac{\partial c_{\mathbf{k}}(t)}{\partial t} = \left[c_{\mathbf{k}}(t), \widehat{H} \right]. \tag{3.4}$$

To evaluate the commutator, we note that since $\widehat{H}$ commutes with itself,

$$\left[c_{\mathbf{k}}\left(t\right),\widehat{H}\right] = \left[c_{\mathbf{k}}\left(t\right), e^{i\widehat{H}t}\widehat{H}e^{-i\widehat{H}t}\right] = \left[c_{\mathbf{k}}\left(t\right), e^{i\widehat{H}t}\left(\sum_{\mathbf{k}'}\epsilon_{\mathbf{k}'}c_{\mathbf{k}'}^{\dagger}c_{\mathbf{k}'}\right)e^{-i\widehat{H}t}\right] \quad (3.5)$$

$$= \left[c_{\mathbf{k}}\left(t\right),\left(\sum_{\mathbf{k}'}\epsilon_{\mathbf{k}'}c_{\mathbf{k}'}^{\dagger}\left(t\right)c_{\mathbf{k}'}\left(t\right)\right)\right] = \sum_{\mathbf{k}'}\epsilon_{\mathbf{k}'}\left[c_{\mathbf{k}}\left(t\right),c_{\mathbf{k}'}^{\dagger}\left(t\right)c_{\mathbf{k}'}\left(t\right)\right]. \quad (3.6)$$

Commutator identities: The following are very useful identities to get equations of motions, and in general equal-time commutators.

$$[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA \quad (3.7)$$

$$\boxed{[A, BC] = [A, B]C + B[A, C]} \quad (3.8)$$

$$\boxed{[A, BC] = \{A, B\}C - B\{A, C\}} \quad (3.9)$$

The first commutator identity is familiar from elementary quantum mechanics. The last one can be memorized by noting that it behaves as if the B had anticommuted with the A.

The above identities can then be used to evaluate the needed commutator either for fermions

$$\left[c_{\mathbf{k}}\left(t\right),c_{\mathbf{k}'}^{\dagger}\left(t\right)c_{\mathbf{k}'}\left(t\right)\right] = \left\{c_{\mathbf{k}}\left(t\right),c_{\mathbf{k}'}^{\dagger}\left(t\right)\right\}c_{\mathbf{k}'}\left(t\right) + 0 = \delta_{\mathbf{k},\mathbf{k}'}c_{\mathbf{k}}\left(t\right) \quad (3.10)$$

or for bosons

$$\left[c_{\mathbf{k}}\left(t\right),c_{\mathbf{k}'}^{\dagger}\left(t\right)c_{\mathbf{k}'}\left(t\right)\right] = \left[c_{\mathbf{k}}\left(t\right),c_{\mathbf{k}'}^{\dagger}\left(t\right)\right]c_{\mathbf{k}'}\left(t\right) + 0 = \delta_{\mathbf{k},\mathbf{k}'}c_{\mathbf{k}}\left(t\right) \quad (3.11)$$

in either case then, the equation of motion becomes

$$i\frac{\partial c_{\mathbf{k}}\left(t\right)}{\partial t} = \left[c_{\mathbf{k}}\left(t\right),\widehat{H}\right] = \epsilon_{\mathbf{k}}c_{\mathbf{k}}\left(t\right) \quad (3.12)$$

whose solution is

$$\boxed{c_{\mathbf{k}}\left(t\right) = e^{-i\epsilon_{\mathbf{k}}t}c_{\mathbf{k}}} \quad (3.13)$$

Taking the adjoint,

$$\boxed{c_{\mathbf{k}}^{\dagger}\left(t\right) = c_{\mathbf{k}}^{\dagger}e^{i\epsilon_{\mathbf{k}}t}}. \quad (3.14)$$

If we had been working in a basis where $\widehat{H}$ was not diagonal, then repeating the steps above,

$$i\frac{\partial a_{\alpha}\left(t\right)}{\partial t} = \left[a_{\alpha}\left(t\right),\widehat{H}\right] = \sum_{\beta,\gamma}\langle\beta|\,\widehat{H}\,|\gamma\rangle\left[a_{\alpha}\left(t\right),a_{\beta}^{\dagger}\left(t\right)a_{\gamma}\left(t\right)\right] = \sum_{\gamma}\langle\alpha|\,\widehat{H}\,|\gamma\rangle\,a_{\gamma}\left(t\right)$$
$$(3.15)$$

whose solution is found by diagonalizing, integrating, and changing back the basis.

3.1 Motivation of the definition of the second quantized Green's function G^{R}

When the Hamiltonian is quadratic in creation-annihilation operators, in other words when we have a one-body problem, the retarded single-particle Green's

function we are about to define does reduce to the Green's function we studied in the one-body Schrödinger equation. Its actual definition is however better suited for many-body problems as we shall see in the present section.

Consider the definition we had before

$$G^R (\mathbf{r},t;\mathbf{r}',t') = -i \langle \mathbf{r}| e^{-iH(t-t')} |\mathbf{r}'\rangle \theta (t - t'). \qquad (3.16)$$

Since in second-quantization the operator $\psi^\dagger (\mathbf{r})$ creates a particle at point $\mathbf{r}$, the following definition seems natural

$$G^R (\mathbf{r},t;\mathbf{r}',t') = -i \langle GS| \psi (\mathbf{r}) e^{-iH(t-t')} \psi^\dagger (\mathbf{r}') |GS\rangle \theta (t - t') \qquad (3.17)$$

In this expression, $|GS\rangle$ is a many-body vacuum (ground-state). Choosing appropriately the zero of energy, $H |GS\rangle = 0 |GS\rangle = 0$ so that the above result could be written

$$G^R (\mathbf{r},t;\mathbf{r}',t') = -i \langle GS| \psi (\mathbf{r},t) \psi^\dagger (\mathbf{r}',t') |GS\rangle \theta (t - t'). \qquad (3.18)$$

This is not quite what we want except in the case where there is a single particle propagating. Indeed, to keep the physical definition of the propagator, it is convenient to have at time $t = t' + 0^+$

$$G^R (\mathbf{r},t + 0^+;\mathbf{r}',t) = -i\delta (\mathbf{r} - \mathbf{r}') \qquad (3.19)$$

reflecting the fact that the wave-function does not have the time to evolve in an infinitesimal time. However, in the present case, the many-body vacuum $|GS\rangle$ is a linear combination of Slater determinants,

$$|GS\rangle = \int d\mathbf{r}_1... \int d\mathbf{r}_N \Psi (\mathbf{r}_1...\mathbf{r}_N) \psi^\dagger (\mathbf{r}_1) ...\psi^\dagger (\mathbf{r}_N) |0\rangle \qquad (3.20)$$

where $\Psi (\mathbf{r}_1...\mathbf{r}_N)$ reduces to the Schrödinger wave function and $|0\rangle$ is a real vacuum. This means that $\langle GS| \psi (\mathbf{r},t) \psi^\dagger (\mathbf{r}',t) |GS\rangle$ is not in general a delta function. This is a manifestation of the fact that we have a many-body problem and that particles are indistinguishable.

Nevertheless, we can recover the desired simple initial condition Eq.(3.19) even in the Many-Body case by adopting the following *definition,* which in a way takes into account the fact that not only electrons, but also holes can now propagate:

$$G^R (\mathbf{r},t;\mathbf{r}',t') = -i \langle GS| \left\{ \psi (\mathbf{r},t) , \psi^\dagger (\mathbf{r}',t') \right\} |GS\rangle \theta (t - t') \quad ; \quad \text{for} \quad \text{fermions} \qquad (3.21)$$

$$G^R (\mathbf{r},t;\mathbf{r}',t') = -i \langle GS| \left[\psi (\mathbf{r},t) , \psi^\dagger (\mathbf{r}',t') \right] |GS\rangle \theta (t - t') \quad ; \quad \text{for} \quad \text{bosons} \qquad (3.22)$$

This is the zero-temperature definition. At finite temperature, the ground-state expectation value is replaced by a thermodynamic average. Hence we shall in general work with

Definition 5

$$\boxed{G^R (\mathbf{r},t;\mathbf{r}',t') = -i \left\langle \left\{ \psi (\mathbf{r},t) , \psi^\dagger (\mathbf{r}',t') \right\} \right\rangle \theta (t - t') \quad ; \quad \textit{for} \quad \textit{fermions}} \qquad (3.23)$$

$$\boxed{G^R (\mathbf{r},t;\mathbf{r}',t') = -i \left\langle \left[\psi (\mathbf{r},t) , \psi^\dagger (\mathbf{r}',t') \right] \right\rangle \theta (t - t') \quad ; \quad \textit{for} \quad \textit{bosons}} \qquad (3.24)$$

These definitions have the desired property that at $t = t' + 0^+$, we have that $G^R (\mathbf{r},t + 0^+;\mathbf{r}',t) = -i\delta (\mathbf{r} - \mathbf{r}')$ as follows from commutation or anti-commutation relations

Remark 26 *Analogies: This definition is now analogous to $\chi^R = 2i\chi"\,\theta\,(t - t')$ which we had in linear response. The imaginary part of the Green's function will again be a commutator or an anticommutator and hence will obey sum-rules.*

Remark 27 *Green's function as a response function: Physically, this definition makes obvious that the Green's function is the response to an external probe which couples linearly to creation-annihilation operators. In the case of fermions, the external probe has to be an anticommuting number (a Grassmann variable, as we shall discuss later).*

3.1.1 Examples with quadratic Hamiltonians:

When the Hamiltonian is quadratic in creation-annihilation operators, the equation of motion obeyed by this Green's function is the same as in the one-body case. An example of quadratic Hamiltonian is that for free particles

$$\langle \mathbf{r}|\, H \,|\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m}\,\langle \mathbf{r}\,|\mathbf{r}_1\rangle = -\frac{\nabla^2}{2m}\delta\,(\mathbf{r} - \mathbf{r}_1)\,. \tag{3.25}$$

In the general second quantized case, we write

$$\widehat{H} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi^\dagger\,(\mathbf{r}_2,t)\,\langle \mathbf{r}_2|\, H \,|\mathbf{r}_1\rangle\,\psi\,(\mathbf{r}_1,t) \tag{3.26}$$

We give two calculations of the Green's function, one directly from the definition and one from the equations of motion (Schrödinger's equation).

Calculation from the definition. For a *quadratic Hamiltonian*, one can also compute directly the Green's function from its definition since, if $|n\rangle$ is an eigenbasis, $\phi_n\,(\mathbf{r}) = \langle \mathbf{r}\,|n\rangle$, $\langle n'|\, H \,|n\rangle = E_n\delta_{n,n'}$

$$\psi\,(\mathbf{r},t) = \sum_n \langle \mathbf{r}\,|n\rangle\,a_n\,(t) = \sum_n e^{-iE_n t}\,\langle \mathbf{r}\,|n\rangle\,a_n = \sum_n e^{-iE_n t}\phi_n\,(\mathbf{r})\,a_n$$
$$\tag{3.27}$$

$$\left\{\psi\,(\mathbf{r},t)\,,\psi^\dagger\,(\mathbf{r}',0)\right\} = \sum_n \sum_m e^{-iE_n t}\phi_n\,(\mathbf{r})\left\{a_n, a_m^\dagger\right\}\phi_m^*\,(\mathbf{r}') = \sum_n e^{-iE_n t}\phi_n\,(\mathbf{r})\,\phi_n^*\,(\mathbf{r}')$$
$$\tag{3.28}$$

$$G^R\,(\mathbf{r},t;\mathbf{r}',0) = -i\left\langle\left\{\psi\,(\mathbf{r},t)\,,\psi^\dagger\,(\mathbf{r}',0)\right\}\right\rangle\theta\,(t) = -i\sum_n e^{-iE_n t}\phi_n\,(\mathbf{r})\,\phi_n^*\,(\mathbf{r}')\,\theta\,(t)$$
$$\tag{3.29}$$

$$G^R\,(\mathbf{r},\mathbf{r}';\omega) = \int dt e^{i(\omega+i\eta)t}\,(-i)\sum_n e^{-iE_n t}\phi_n\,(\mathbf{r})\,\phi_n^*\,(\mathbf{r}')\,\theta\,(t) = \sum_n \frac{\phi_n\,(\mathbf{r})\,\phi_n^*\,(\mathbf{r}')}{\omega + i\eta - E_n}$$
$$\tag{3.30}$$

Calculation from the equations of motion In general, the equation of motion can be obtained as follows

$$i\frac{\partial}{\partial t}G^R\,(\mathbf{r},t;\mathbf{r}',t') = i\frac{\partial}{\partial t}\left[-i\left\langle\left\{\psi\,(\mathbf{r},t)\,,\psi^\dagger\,(\mathbf{r}',t')\right\}\right\rangle\theta\,(t - t')\right] \tag{3.31}$$

$$= \left\langle\left\{\psi\,(\mathbf{r},t)\,,\psi^\dagger\,(\mathbf{r}',t')\right\}\right\rangle\delta\,(t - t') + i\left\langle\left\{\left[\widehat{H},\psi\,(\mathbf{r},t)\right],\psi^\dagger\,(\mathbf{r}',t')\right\}\right\rangle\theta\,(t - t')$$
$$\tag{3.32}$$

Following the steps analogous to those in Eq.(3.10) above, using the anti-commutation relations Eqs.(**??**)(**??**) it is clear that

$$\left[\widehat{H}, \psi\left(\mathbf{r},t\right)\right] = -\int d\mathbf{r}_1 \left\langle \mathbf{r}\right| H \left|\mathbf{r}_1\right\rangle \psi\left(\mathbf{r}_1,t\right) \tag{3.33}$$

so that

$$i\frac{\partial}{\partial t} G^R\left(\mathbf{r},t;\mathbf{r}',t'\right) \tag{3.34}$$

$$= \delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) - i\int d\mathbf{r}_1 \left\langle \mathbf{r}\right| H \left|\mathbf{r}_1\right\rangle \left\langle \left\{\psi\left(\mathbf{r}_1,t\right), \psi^\dagger\left(\mathbf{r}',t'\right)\right\}\right\rangle \theta\left(t-t'\right)$$

$$= \delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) + \int d\mathbf{r}_1 \left\langle \mathbf{r}\right| H \left|\mathbf{r}_1\right\rangle G^R\left(\mathbf{r}_1,t;\mathbf{r}',t'\right) \tag{3.35}$$

This last expression may be rewritten as

$$\int d\mathbf{r}_1 \left\langle \mathbf{r}\right| i\frac{\partial}{\partial t} - \widehat{H} \left|\mathbf{r}_1\right\rangle G^R\left(\mathbf{r}_1,t;\mathbf{r}',t'\right) = \delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) \tag{3.36}$$

$$= \left\langle \mathbf{r}\left|\mathbf{r}'\right\rangle \delta\left(t-t'\right) \tag{3.37}$$

where we recognize the equation (**??**) found in the previous Chapter. Formally then

$$\left\langle \mathbf{r}\right| \left(i\frac{\partial}{\partial t} - \widehat{H}\right) G^R\left(t-t'\right) \left|\mathbf{r}'\right\rangle = \left\langle \mathbf{r}\left|\mathbf{r}'\right\rangle \delta\left(t-t'\right) \tag{3.38}$$

so that the operator form of the Green's function is the same as that found before, namely

$$\widehat{G}^R\left(t-t'\right) = \left(i\frac{\partial}{\partial t} - \widehat{H}\right)^{-1}\delta\left(t-t'\right) \tag{3.39}$$

It is convenient to rewrite the result for the equation of motion Eq.(3.36) in the following form that is more symmetrical in space and time.

$$\int d\mathbf{r}_1 \int dt_1 \left\langle \mathbf{r}\right| i\frac{\partial}{\partial t} - \widehat{H} \left|\mathbf{r}_1\right\rangle \delta\left(t-t_1\right) G^R\left(\mathbf{r}_1,t_1;\mathbf{r}',t'\right) = \delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) \tag{3.40}$$

We may as well let time play a more important role since in the many-body case it will be essential, as we have already argued in the context of the frequency dependence of the self-energy. The inverse of the Green's function in this notation is just like above,

$$G^R\left(\mathbf{r},t;\mathbf{r}_1,t_1\right)^{-1} = \left\langle \mathbf{r}\right| i\frac{\partial}{\partial t} - \widehat{H} \left|\mathbf{r}_1\right\rangle \delta\left(t-t_1\right). \tag{3.41}$$

Seen from this point of view, the integrals over time and space are the continuum generalization of matrix multiplication. The delta function is like the identity matrix.

Definition 6 *The following short-hand notation is often used*

$$\boxed{G^R\left(1,1'\right) \equiv G^R\left(\mathbf{r},t;\mathbf{r}',t'\right)} \tag{3.42}$$

$$\boxed{G^R\left(1,\bar{1}\right)^{-1} G^R\left(\bar{1},1'\right) = \delta\left(1-1'\right)} \tag{3.43}$$

where the index with the overbar stands for an integral.

MOTIVATION OF THE DEFINITION OF THE SECOND QUANTIZED GREEN'S FUNCTION G^R

3.2 Interaction representation and time-ordered product

Perturbation theory in the many-body case is less trivial than in the one-body case. In the many-body case time and frequency dependence are unavoidable. To construct perturbation theory we will follow the same steps as those used in the derivation of linear response theory. The only difference is that we will write a formally exact solution for the evolution operator in the interaction representation instead of using only the first order result. The important concept of time-ordered product comes out naturally from this exercise.

The plan is to recall the Heisenberg and Schrödinger pictures, and then to introduce the interaction representation in the case where the Hamiltonian can be written in the form

$$H = H_0 + V \tag{3.44}$$

where

$$[H_0, V] \neq 0 \tag{3.45}$$

Let us begin. We assume that H is time independent. Typical matrix elements we want to compute at finite temperature are of the form

$$\langle i | e^{-\beta H} \psi_H(t) \psi_H^\dagger(t') | i \rangle \tag{3.46}$$

We do not write explicitly indices other than time to keep the notation simple. Recall the Heisenberg and Schrödinger picture

$$\psi_H(t) = e^{iHt} \psi_S e^{-iHt} \tag{3.47}$$

We define the time evolution operator

$$U(t, 0) = e^{-iHt} \tag{3.48}$$

so that

$$\psi_H(t) = U(0, t) \psi_S U(t, 0) \tag{3.49}$$

Because from now on we assume time-reversal symmetry, we will always make the replacement

$$U^\dagger(t, 0) = U(0, t) \tag{3.50}$$

as we just did. The differential equation for the time-evolution operator is

$$i\frac{\partial U(t, 0)}{\partial t} = HU(t, 0) \tag{3.51}$$

With the initial condition $U(0, 0) = 1$ it has $U(t, 0) = e^{-iHt}$ as its solution. It obeys the semi-group property

$$U(t, t') = U(t, 0) U(0, t') = e^{-iH(t-t')} \tag{3.52}$$

$$U^{-1}(t, 0) = U(0, t) \tag{3.53}$$

$$U(t_0, t_0) = 1 \tag{3.54}$$

for arbitrary t_0

We are now ready to introduce the interaction representation. In this representation, the fields evolve with the unperturbed Hamiltonian

$$\boxed{\widehat{\psi}\left(t\right) = e^{iH_0 t}\psi_S e^{-iH_0 t}} \tag{3.55}$$

Note that we now use the caret (hat) to mean "interaction picture". We hope this change of notation causes no confusion. To introduce these interaction representation fields in a general matrix element,

$$\langle i| e^{-\beta H}\psi_H\left(t\right)\psi_H^\dagger\left(t'\right)|i\rangle = \langle i| e^{-\beta H} U\left(0,t\right)\psi_S U\left(t,0\right) U\left(0,t'\right)\psi_S^\dagger U\left(t',0\right)|i\rangle \tag{3.56}$$

it suffices to notice that it is easy to remove the extra $e^{iH_0 t}$ coming from the replacement of ψ_S by $e^{-iH_0 t}\widehat{\psi}\left(t\right)e^{iH_0 t}$ simply by including them in the definition of the evolution operator in the interaction representation

$$\widehat{U}\left(t,0\right) = e^{iH_0 t}U\left(t,0\right) \tag{3.57}$$

$$\widehat{U}\left(0,t\right) = U\left(0,t\right)e^{-iH_0 t} \tag{3.58}$$

$$\widehat{U}\left(t,0\right)\widehat{U}\left(0,t\right) = \widehat{U}\left(0,t\right)\widehat{U}\left(t,0\right) = 1 \tag{3.59}$$

With these definitions, we have that our general matrix element takes the form

$$\langle i| e^{-\beta H}\psi_H\left(t\right)\psi_H^\dagger\left(t'\right)|i\rangle = \langle i| e^{-\beta H}\widehat{U}\left(0,t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t,0\right)\widehat{U}\left(0,t'\right)\widehat{\psi}^\dagger\left(t'\right)\widehat{U}\left(t',0\right)|i\rangle \tag{3.60}$$

The purpose of the exercise is evidently to find a perturbation expansion for the evolution operator in the interaction representation. It will be built starting from its equation of motion

$$i\frac{\partial\widehat{U}\left(t,0\right)}{\partial t} = e^{iH_0 t}\left(-H_0 + H\right) U\left(t,0\right) = e^{iH_0 t}V\quad \left(e^{-iH_0 t}e^{iH_0 t}\right)\quad U\left(t,0\right)\tag{3.61}$$

Since a general operator is a product of ψ fields, it will also evolve with time in the same way so it is natural to define the interaction representation for V as well. Our final result for the equation of motion for $\widehat{U}\left(t,0\right)$ is then

$$i\frac{\partial\widehat{U}\left(t,0\right)}{\partial t} = \widehat{V}\left(t\right)\widehat{U}\left(t,0\right)$$

Multiplying on the right by $\widehat{U}\left(0,t_0\right)$ we have a more general equation

$$\boxed{i\frac{\partial\widehat{U}(t,t_0)}{\partial t} = \widehat{V}\left(t\right)\widehat{U}\left(t,t_0\right)} \tag{3.62}$$

Remark 28 *Difficulties associated with the fact that we have non-commuting operators: The solution of this equation is not $e^{-i\int \widehat{V}(t)dt}$. We will see momentarily how the real solution looks formally like an exponential while at the same time being very different from it. To write the solution as a simple exponential is wrong because it assumes that we can manipulate $\widehat{U}\left(t,t_0\right)$ as if it was a number. In reality it is an operator so that $\frac{\partial\widehat{U}(t,t_0)}{\partial t}\widehat{U}\left(t,t_0\right)^{-1} \neq \frac{\partial}{\partial t}\ln\widehat{U}\left(t,t_0\right)$. Indeed, note the ambiguity in writing the definition of this derivative: Should we write*

$$\frac{\partial}{\partial t}\ln\widehat{U}\left(t,t_0\right) = \lim_{\Delta t \to 0}\widehat{U}\left(t,t_0\right)^{-1}\left[\widehat{U}\left(t+\Delta t,t_0\right) - \widehat{U}\left(t,t_0\right)\right]/\Delta t$$

or

$$\lim_{\Delta t \to 0}\left[\widehat{U}\left(t+\Delta t,t_0\right) - \widehat{U}\left(t,t_0\right)\right]\widehat{U}\left(t,t_0\right)^{-1}/\Delta t \text{ ?} \tag{3.63}$$

The two limits cannot be identical since in general

$$\lim_{\Delta t \to 0} \left[\widehat{U}\left(t + \Delta t, t_0\right), \widehat{U}\left(t, t_0\right)^{-1} \right] \neq 0. \tag{3.64}$$

because $\widehat{U}\left(t, t_0\right)$ is made up of operators such as V and e^{-iH_0t} that do not commute with each other.

To solve the equation for the evolution operator Eq.(3.62), it is more convenient to write the equivalent integral equation that is then solved by iteration. Integration on both sides of the equation and use of the initial condition Eq.(3.54) gives immediately

$$\int_{t_0}^{t} \frac{\partial \widehat{U}\left(t', t_0\right)}{\partial t'} dt' = -i \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \widehat{U}\left(t', t_0\right) \tag{3.65}$$

$$\widehat{U}\left(t, t_0\right) = 1 - i \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \widehat{U}\left(t', t_0\right) \tag{3.66}$$

Solving by iteration, we find

$$\widehat{U}\left(t, t_0\right) = 1 - i \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \widehat{U}\left(t', t_0\right) = \tag{3.67}$$

$$= 1 - i \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) + (-i)^2 \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \int_{t_0}^{t'} dt'' \widehat{V}\left(t''\right) \tag{3.68}$$

$$+ (-i)^3 \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \int_{t_0}^{t'} dt'' \widehat{V}\left(t''\right) \int_{t_0}^{t''} dt''' \widehat{V}\left(t'''\right) + ... \tag{3.69}$$

Suppose $t > t_0$ and consider a typical term in this series. By suitably defining a contour C and time-ordering operator along this contour T_c, it can be rearranged as follows

$$(-i)^3 \int_{t_0}^{t} dt' \widehat{V}\left(t'\right) \int_{t_0}^{t'} dt'' \widehat{V}\left(t''\right) \int_{t_0}^{t''} dt''' \widehat{V}\left(t'''\right) \tag{3.70}$$

$$= (-i)^3 \frac{1}{3!} T_c \left[\int_C dt_1 \widehat{V}\left(t_1\right) \int_C dt_2 \widehat{V}\left(t_2\right) \int_C dt_3 \widehat{V}\left(t_3\right) \right] \tag{3.71}$$

where

- C is a contour that is here just a real line segment going from t_0 to t.

- T_c is the "time-ordering operator". Assuming $t > t_0$, *it places the operator which appear later on the contour C to the left*. For the time being, T_c orders operators that are bosonic in nature. A generalization will appear soon with fermionic Green's functions.

- The integral on the lef-hand side of the last equation covers all possible times such that the operators with the time that is largest (latest) are to the left. The $\frac{1}{3!}$ comes from the fact that for a general $\widehat{V}\left(t_1\right) \widehat{V}\left(t_2\right) \widehat{V}\left(t_3\right)$ there are 3! ways of ordering the operators. All these possible orders appear in the integrals on the right-hand side of the last equation. The operator T_c always orders them in the order corresponding to the left-hand side, but this means that the integral on the left-hand side appears 3! times on the right-hand side, hence the overall factor of $\frac{1}{3!}$.

- A product of operators on which T_c acts is called a time-ordered product.

One also needs $\widehat{U}(0,t)$. In this case, with $t > 0$, the operators at the earliest time are on the left. This means that the contour on which the T_c is defined is ordered along the opposite direction.

A general term of the series may thus be written as

$$\widehat{U}(t,t_0) = \sum_{k=0}^{\infty} (-i)^k \frac{1}{k!} T_c \left[\left(\int_C dt_1 \widehat{V}(t_1) \right)^k \right] \tag{3.72}$$

which we can in turn write in the convenient notation

$$\boxed{\widehat{U}(t,t_0) = T_c \left[\exp \left(-i \int_C dt_1 \widehat{V}(t_1) \right) \right]} \tag{3.73}$$

where the contour is as defined above. In other words, operators are ordered right to left from t_0 to t whether t, as a real number, is larger or smaller than t_0.

We can check the limiting case $[H_0, V] = 0$. Then $\widehat{V}$ is independent of time and we recover the expected exponential expression for the time evolution operator.

The definition of the time-ordering operator is extremely useful in practice not only as a formal device that allows the time evolution to still look like an exponential operator (which is explicitly unitary) but also because in many instances it will allow us to treat operators on which it acts as if they were ordinary numbers.

In the zero-temperature formalism, the analog of $\widehat{U}(t,t_0)$ is the so-called S matrix. The time-ordering concept is due to Feynman and Dyson.

Remark 29 *Non-quadratic unperturbed Hamiltonians: It is important to notice that in everything above, H_0 does not need to be quadratic in creation-annihilation operators. With very few exceptions however,[10] it is quadratic since we want the "unperturbed" Hamiltonian to be easily solvable. Note that the case where H_0 is time dependent can also be treated but in this case we would have an evolution operator $U_0(t,0)$ instead of $e^{-iH_0 t}$. The only property of the exponential that we really use in the above derivation is the composition law obeyed by time-evolution operators in general, namely $U_0(t,t') U_0(t',t'') = U_0(t,t'')$.*

Remark 30 *The general case of time-dependent Hamiltonians: The problem we just solved for the time evolution in the interaction picture Eq.(3.62) is a much more general problem that poses itself whenever the Hamiltonian is time-dependent.*

3.3 Kadanoff-Baym and Keldysh-Schwinger contours

While we have discussed only the time evolution of the operators in the interaction representation, it is clear that we should also take into account the fact that the density matrix $e^{-\beta H}$ should also be calculated with perturbative methods. The results of the previous section can trivially be extended to the density matrix by a simple analytic continuation $t \to -i\tau$. In doing so in the present section, we will discover the many advantages of imaginary time for statistical mechanics.

Let us define evolution operators and the interaction representation for the density matrix in basically the same way as before

$$e^{-\beta H} = U(-i\beta, 0) = e^{-iH_0(-i\beta)} \widehat{U}(-i\beta, 0) = e^{-\beta H_0} \widehat{U}(-i\beta, 0) \tag{3.74}$$

The solution of the imaginary time evolution equation

$$i \frac{\partial \widehat{U}(it'', 0)}{\partial (it'')} = \widehat{V}(it'') \widehat{U}(it'', 0)$$

is then

$$\widehat{U}\left(-i\beta,0\right)=T_c\left[\exp\left(-i\int_C d\left(it''\right)\widehat{V}\left(it''\right)\right)\right] \tag{3.75}$$

where

$$\boxed{t'' \equiv \mathrm{Im}\left(t\right)} \tag{3.76}$$

$$\widehat{V}\left(it''\right)=e^{-t''H_0}Ve^{t''H_0} \tag{3.77}$$

and the contour C now proceeds from $t''=0$ to $t''=-\beta$.

Overall now, the matrix elements that we need to evaluate can be expressed in such a way that the trace will be performed over the unperturbed density matrix. Indeed, using our above results, we find

$$\langle i|\,e^{-\beta H}\psi_H\left(t\right)\psi_H^+\left(t'\right)|i\rangle = \langle i|\,e^{-\beta H_0}\widehat{U}\left(-i\beta,0\right)\widehat{U}\left(0,t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t,0\right)\widehat{U}\left(0,t'\right)\widehat{\psi}^+\left(t'\right)\widehat{U}\left(t',0\right)|i\rangle \tag{3.78}$$

We want to take initial states at a time t_0 so that in practical calculations where the system is *out of equilibrium* we can choose $t_0=-\infty$ where we can assume that the system is in equilibrium at this initial time. Hence, we are here considering a more general case than we really need but that is not more difficult so let us continue. Since we are evaluating a trace, we are free to take

$$|i\rangle = \widehat{U}\left(0,t_0\right)|i\left(t_0\right)\rangle \tag{3.79}$$

then we have

$$\langle i|\,e^{-\beta H} = \langle i\left(t_0\right)|\,\widehat{U}\left(t_0,0\right)e^{-\beta H} = \langle i\left(t_0\right)|\left(e^{-\beta H_0}e^{\beta H_0}\right)\left(e^{iH_0t_0}e^{-iHt_0}\right)e^{-\beta H} \tag{3.80}$$

$$= \langle i\left(t_0\right)|\,e^{-\beta H_0}e^{iH_0\left(t_0-i\beta\right)}e^{-iH\left(t_0-i\beta\right)} = \langle i\left(t_0\right)|\,e^{-\beta H_0}\widehat{U}\left(t_0-i\beta,0\right) \tag{3.81}$$

This allows us to write an arbitrary matrix element entering the thermodynamic trace as the evolution along a contour in complex time

$$\langle i|\,e^{-\beta H}\psi_H\left(t\right)\psi_H^\dagger\left(t'\right)|i\rangle = \langle i\left(t_0\right)|\,e^{-\beta H_0}\widehat{U}\left(t_0-i\beta,0\right)\widehat{U}\left(0,t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t,0\right)\widehat{U}\left(0,t'\right)\widehat{\psi}^\dagger\left(t'\right)\widehat{U}\left(t',0\right)|i\rangle$$

$$= \langle i\left(t_0\right)|\,e^{-\beta H_0}\widehat{U}\left(t_0-i\beta,t_0\right)\widehat{U}\left(t_0,t\right)\widehat{\psi}\left(t\right)\widehat{U}\left(t,t'\right)\widehat{\psi}^\dagger\left(t'\right)\widehat{U}\left(t',t_0\right)|i\left(t_0\right)\rangle \quad \text{(3.82)}$$

How would we evaluate the retarded Green's function in practice using this approach? Take the case of fermions. It is convenient to define $G^>\left(t-t'\right)$ and $G^<\left(t-t'\right)$ by

$$\boxed{G^>\left(t-t'\right)=-i\left\langle\psi_H\left(t\right)\psi_H^\dagger\left(t'\right)\right\rangle} \tag{3.83}$$

$$\boxed{G^<\left(t-t'\right)=i\left\langle\psi_H^\dagger\left(t'\right)\psi_H\left(t\right)\right\rangle} \tag{3.84}$$

in such a way that

$$G^R\left(t-t'\right)=-i\left\langle\left\{\psi_H\left(t\right),\psi_H^\dagger\left(t'\right)\right\}\right\rangle\theta\left(t-t'\right)\equiv\left[G^>\left(t-t'\right)-G^<\left(t-t'\right)\right]\theta\left(t-t'\right) \tag{3.85}$$

To evaluate $G^>\left(t-t'\right)$ for example, we would expand the evolution operators such as $\widehat{U}\left(t',t_0\right)$ as a power series in $\widehat{V}$, each power of $\widehat{V}$ being associated with an integral of a time ordered product that would start from t_0 to go to the creation operator $\widehat{\psi}^\dagger\left(t'\right)$, then go to the destruction operator $\widehat{\psi}\left(t\right)$ until it returns to $t_0-i\beta$. This contour is illustrated in Fig.(3-1). It is this contour that determines the order of the operators, so that even if t' is a larger number than t, as illustrated on the right panel of this figure, the operator $\widehat{\psi}\left(t\right)$ always occur after $\widehat{\psi}^\dagger\left(t'\right)$ on the
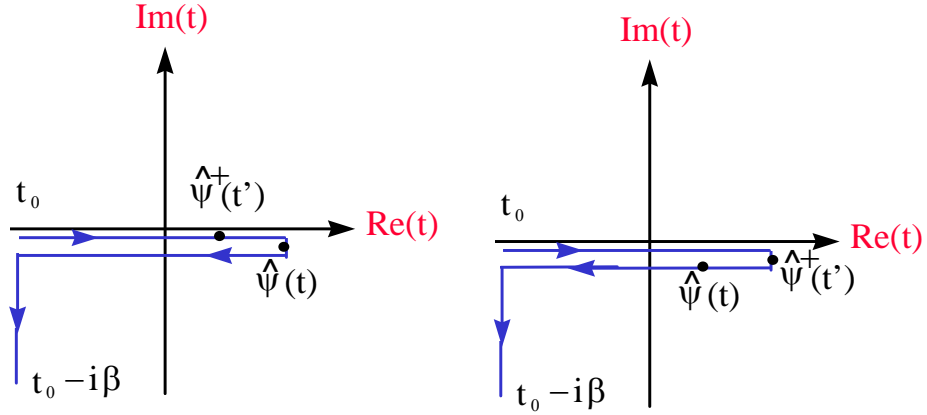
Figure 3-1   Kadanoff-Baym contour to compute $G^> (t - t')$.

contour, *i.e.* $\widehat{\psi}(t)$ is on the left of $\widehat{\psi}^{\dagger}(t')$ in the algebraic expression. The parts of the contour that follow the real axis are displaced slightly along the imaginary direction for clarity.

We will see momentarily that it is possible to avoid this complicated contour to make calculations of equilibrium quantities. However, in non-equilibrium situations, such contours are unavoidable. In practice however, what is used by most authors is the Keldysh-Schwinger contour that is obtained by inserting $\widehat{U}(t', \infty)\widehat{U}(\infty, t') = 1$ to the left of $\widehat{\psi}^{\dagger}(t')$ in the algebraic expression Eq.(3.82). In practice this greatly simplifies the calculations since the contour, illustrated in Fig.(3-2), is such that integrals always go from $-\infty$ to ∞. To specify if a given creation or annihilation operator is on the upper or the lower contour, a simple 2×2 matrix suffices since there are only four possibilities..
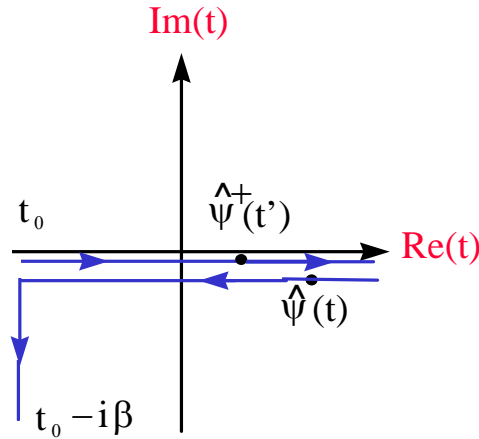
Figure 3-2   Keldysh-Schwinger contour.

In equilibrium, the analog of the fluctuation dissipation theorem in the form of Eq.(2.125) for correlation functions, allows us to relate $G^>$ and $G^<$, which means that we can simplify matters greatly and work with a single Green function. Fundamentally, this is what allows us to introduce in the next section a simpler contour that is extremely more convenient for systems in equilibrium, and hence for linear response.

3.4 Matsubara Green's function and its relation to usual Green's functions. (The case of fermions)

In thermodynamic equilibrium the time evolution operator as well as the density matrix are exponentials of H times a complex number. To evaluate these operators perturbatively, one needs to calculate time-ordered products along a contour in the complex time domain that is relatively complicated, as we saw in the previous section. In the present section, we introduce a Green's function that is itself a time-ordered product but along the imaginary time axis only, as illustrated in Fig.(3-3) below. This slight generalization of the Green's function is a mathematical device that is simple, elegant and extremely convenient since the integration contour is now simple. In a sense, we take advantage of the fact that we are free to define Green functions as we wish, as long as we connect them to observable quantities in the corresponding manner at the end of the calculation. What makes this Green function extremely useful for calculations is the fact that in evaluating time-ordered products that occur in the perturbation series, a theorem (Wick's theorem) tells us that all correlations functions are related to producs of time-ordered Green's functions. So we might as well focus on this quantity from the start. For thermodynamic quantities, since only equal-time correlation functions are needed, it is clear that evaluation in imaginary time or in real time should be equivalent since only $t = 0$ is relevant. More generally, for time-dependent correlation functions we will see that in frequency space the analytic continuation to the physically relevant object, namely the retarded function, is trivial. Also, the same tricks apply not only to Green's functions but also to general response functions such as the density-density correlation function.

After introducing the so-called Matsubara Green's function itself, we will study its properties. First, using essentially the same trick as for the fluctuation-dissipation theorem for correlation functions, we prove that these functions are antiperiodic in imaginary time. This allows us to expand these functions in a Fourier series. The spectral representation and the so-called Lehman representation then allow us to make a clear connection between the Matsubara Green's function and the retarded function through analytic continuation. As usual, the spectral representation also allows us to do high-frequency expansions. We give specific examples of Matsubara Green's functions for non-interacting particles and show in general how to treat their Fourier series expansions, *i.e.* how to do sums over Matsubara frequencies.

3.4.1 Definition

The Matsubara Green's function is defined by

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau - \tau'\right) = -\left\langle T_\tau \psi\left(\mathbf{r},\tau\right)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle} \qquad (3.86)$$

$$= -\left\langle \psi\left(\mathbf{r},\tau\right)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle \theta\left(\tau - \tau'\right) + \left\langle \psi^\dagger\left(\mathbf{r}',\tau'\right)\psi\left(\mathbf{r},\tau\right)\right\rangle \theta\left(\tau' - \tau\right) \qquad (3.87)$$

The definition of Ref.([11]) has an overall minus sign difference with the definition given here.

Definition 7 *The last equation above defines the time ordering operator for fermions. It is very important to notice the minus sign associated with interchanging*

two fermion operators. This time-ordering operator is thus a slight generalization of the time-ordering operator we encountered before. There was no minus sign in this case associated with the interchange of operators. The time-ordering operator for bosonic quantities, such as V that appeared in the perturbation expansion, will never have a minus sign associated with the exchange of bosonic operators.

We still need to specify a few things. First, the thermodynamic average is in the grand-canonical ensemble

$$\langle \mathcal{O} \rangle \equiv \frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]} \tag{3.88}$$

with μ the chemical potential and N is the total number of particle operator, while the time evolution of the operators is defined by

$$\boxed{\psi\left(\mathbf{r},\tau\right) \equiv e^{\tau(H-\mu N)}\psi_S\left(\mathbf{r}\right)e^{-\tau(H-\mu N)}} \tag{3.89}$$

$$\boxed{\psi^{\dagger}\left(\mathbf{r},\tau\right) \equiv e^{\tau(H-\mu N)}\psi_S^{+}\left(\mathbf{r}\right)e^{-\tau(H-\mu N)}} \tag{3.90}$$

For convenience, it is useful to define

$$\boxed{K \equiv H - \mu N} \tag{3.91}$$

Several points should attract our attention:

- The correspondence with the real time evolution operators e^{-iHt} is done by noting that

$$\tau = -\operatorname{Im}\left(t\right) \tag{3.92}$$

 or, in general for complex time

$$\boxed{\tau = it}$$

- Strictly speaking, we should use $\psi\left(\mathbf{r}, -i\tau\right)$ if we want the symbol $\psi\left(\mathbf{r},t\right)$ for t complex to mean the same thing as before. That is why several authors write $\widehat{\psi}\left(\mathbf{r},\tau\right)$ for the Matsubara field operator. We will stick with $\psi\left(\mathbf{r},\tau\right)$ since this lack of rigor does not usually lead to confusion. We have already given enough different meanings to $\widehat{}$ in previous sections! Furthermore, this type of change of "confusion" in the notation is very common in Physics. For example, we should never write $f\left(\mathbf{k}\right)$ to denote the Fourier transform of $f\left(\mathbf{r}\right)$.

- $\psi^{\dagger}\left(\mathbf{r},\tau\right)$ is *not* the adjoint of $\psi\left(\mathbf{r},\tau\right)$. However, its analytic continuation $\tau \rightarrow it$ is the adjoint of $\psi\left(\mathbf{r},t\right)$.

- Using as usual the cyclic property of the trace, it is clear that $\mathcal{G}$ depends only on $\tau - \tau'$ and not on τ or τ' separately.

- It suffices to define the Matsubara Green's function $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ in the interval $-\beta \leq \tau \leq \beta$. We do not need it outside of this interval. The perturbation expansion of $\widehat{U}\left(-i\beta,0\right) = T_c\left[\exp\left(-\int_C d\tau\widehat{V}\left(\tau\right)\right)\right]$ evidently necessitates that we study at least the interval $0 \leq \tau \leq \beta$ but the other part of the interval, namely $-\beta \leq \tau \leq 0$ is also necessary if we want the time ordering operator to lead to both of the possible orders of ψ and $\psi^{\dagger}$: namely $\psi^{\dagger}$ to the left of ψ and $\psi^{\dagger}$ to the right of ψ. Both possibilities appear in G^R. If we had only $\tau > 0$, only one possibility would appear in the Matsubara Green's function. We will see however in the next section that, in practice, antiperiodicity allows us to trivially take into account what happens in the interval $-\beta \leq \tau \leq 0$ if we know what happens in the interval $0 \leq \tau \leq \beta$.

- The last contour considered in the previous section for $\widehat{U}(-i\beta, 0) = T_c \left[\exp \left(- \int_C d\tau \widehat{V}(\tau) \right) \right]$ tells us that the time-ordering operator T_τ orders along the contour $(\mathrm{Im}(t) = -\beta) > (\mathrm{Im}(t') = \beta)$ which corresponds to $(\tau = \beta) > (\tau' = -\beta)$. The present contour is illustrated in Fig.(3-3).
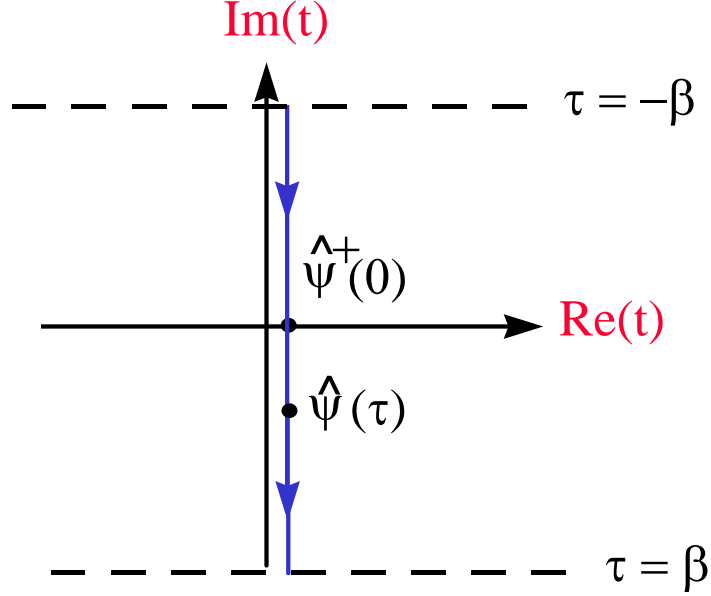
Figure 3-3   Contour for time ordering in imaginary time. Only the time difference is important. The contour is translated slightly along the real-time axis for clarity.

Remark 31 *Role of extra chemical potential in time evolution: The extra chemical potential in the evolution operator $e^{\tau(H-\mu N)}$ is convenient to make all operators, including the density matrix, evolve in the same way. It corresponds to measuring energies with respect to the chemical potential as we will see with the Lehman representation below. The extra $e^{-\tau\mu N}$ disappears for equal-time quantities (thermodynamics) and in the calculation of expectation values $\langle \mathcal{O}^+(t)\mathcal{O}(t') \rangle$ for operators $\mathcal{O}$ which are bilinear in fermions of the form $(\psi^+\psi)$ at equal time. Indeed in that case one has $\mathcal{O}^+(t) = e^{iHt}\mathcal{O}^+e^{-iHt} = e^{i(H-\mu N)t}\mathcal{O}^+e^{-i(H-\mu N)t}$. When Wick's theorem is used to compute expectation values, the creation and annihilation operators evolve then as above. In any case, as we just said, the addition of the chemical potential in the evolution operator just amounts to measuring the single-particle energies with respect to the chemical potential.*

3.4.2   Antiperiodicity and Fourier expansion (Matsubara frequencies)

Suppose $\tau < 0$. Then

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = \left\langle \psi^+(\mathbf{r}', 0) \psi(\mathbf{r}, \tau) \right\rangle \tag{3.93}$$

Using the cyclic property of the trace twice, as in the demonstration of the fluctuation-dissipation theorem it is easy to show that

$$\boxed{\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = -\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau + \beta) \quad ; \quad \tau < 0} \tag{3.94}$$

This boundary condition is sometimes known as the Kubo-Martin-Schwinger (KMS) boundary condition.

Proof: Let

$$e^{-\beta\Omega} \equiv \mathrm{Tr}\left[e^{-\beta K}\right] \tag{3.95}$$

then

$$\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right) = e^{\beta\Omega}\,\mathrm{Tr}\left[e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\left(e^{K\tau}\psi\left(\mathbf{r}\right)e^{-K\tau}\right)\right] \tag{3.96}$$

The cyclic property of the trace then tells us that

$$\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right) = e^{\beta\Omega}\,\mathrm{Tr}\left[\left(e^{K\tau}\psi\left(\mathbf{r}\right)e^{-K\tau}\right)e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\right] \tag{3.97}$$

$$= e^{\beta\Omega}\,\mathrm{Tr}\left[\left(e^{-\beta K}e^{\beta K}\right)\left(e^{K\tau}\psi\left(\mathbf{r}\right)e^{-K\tau}\right)e^{-\beta K}\psi^+\left(\mathbf{r}'\right)\right] \tag{3.98}$$

$$= \left\langle\psi\left(\mathbf{r}, \tau+\beta\right)\psi^+\left(\mathbf{r}', 0\right)\right\rangle \tag{3.99}$$

$$= -\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau+\beta\right) \tag{3.100}$$

The last line follows because given that $-\beta < \tau$, we necessarily have $\tau+\beta > 0$ so that the other θ function must be used in the definition of the Matsubara Green's function.

If $\tau > 0$, the above arguments can be repeated to yield

$$\boxed{\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau-\beta\right) = -\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right)} \quad ; \quad \tau > 0 \tag{3.101}$$

However, for $\tau > 0$ note that

$$\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right) \neq -\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau+\beta\right) \quad ; \quad \tau > 0 \tag{3.102}$$

While $\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau+\beta\right)$ for $\tau > 0$ is well defined, we never need this function. So we restrict ourselves to the interval $-\beta \leq \tau \leq \beta$ described in the previous section.

One can take advantage of the antiperiodicity property of the Green's function in the interval $-\beta \leq \tau \leq \beta$ to expand it in a Fourier series that will automatically guaranty that the crucial antiperiodicity property is satisfied. More specifically, we write

$$\boxed{\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right) = \tfrac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-ik_n\tau}\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; ik_n\right)} \tag{3.103}$$

where the so-called Matsubara frequencies for fermions are odd, namely

$$\boxed{k_n = (2n+1)\,\pi T = \tfrac{(2n+1)\pi}{\beta}} \quad ; \quad n \quad \text{integer} \tag{3.104}$$

The antiperiodicity property will be automatically fulfilled because $e^{-ik_n\beta} = e^{-i(2n+1)\pi} = -1$.

The expansion coefficients are obtained as usual for Fourier series of antiperiodic functions from

$$\boxed{\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; ik_n\right) = \int_0^{\beta} d\tau\, e^{ik_n\tau}\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right)} \tag{3.105}$$

Note that only the $\tau > 0$ region of the domain of definition is needed, as promised.

Remark 32 *Domain of definition of the Matsubara Green's function: The value of $\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau\right)$ given by the Fourier series (3.103) for τ outside the interval $-\beta < \tau < \beta$, is in general different from the actual value of Eq.(3.86) $\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau-\tau'\right) = -\left\langle T_\tau\psi\left(\mathbf{r}, \tau\right)\psi^+\left(\mathbf{r}', \tau'\right)\right\rangle$. Indeed, to define a Fourier series one extends the function defined in the interval $-\beta < \tau < \beta$ so that it is periodic in τ outside this interval with a period 2β. The true function $\mathcal{G}\left(\mathbf{r}, \mathbf{r}'; \tau-\tau'\right) = -\left\langle T_\tau\psi\left(\mathbf{r}, \tau\right)\psi^+\left(\mathbf{r}', \tau'\right)\right\rangle$ has an envelope that is, instead, exponential outside the original interval. We*

will see an explicit example in the case of the free particles. In perturbation ex-
pansions, we never need $\mathcal{G}\left(\mathbf{r}, \mathbf{r}';\tau\right)$ outside the interval where the series and the
true definition give different answers. To avoid mathematical inconsistencies, it is
nevertheless preferable in calculations to do Matsubara frequency sums before any
other integral! It is possible to invert the order of integration and of summation
but we must beware.

3.4.3 Spectral representation, relation between G^R and $\mathcal{G}$ and analytic continuation

By analogy with what we have done previously for response functions χ, it is useful to introduce the spectral representation for the retarded Green's function. We obtain explicitly $\mathcal{G}\left(\mathbf{r}, \mathbf{r}';ik_n\right)$ by integration in the complex plane and find that is trivially related to $G^R\left(\mathbf{r}, \mathbf{r}';\omega\right)$.

As before, we have

$$G^R\left(\mathbf{r}, \mathbf{r}';t\right) = -i\left\langle\left\{\psi\left(\mathbf{r},t\right), \psi^\dagger\left(\mathbf{r}',0\right)\right\}\right\rangle\theta\left(t\right) \tag{3.106}$$

but this time, the evolution operator is defined to take into account the fact that we will work in the grand-canonical ensemble. By analogy with the definition of the Matsubara operators, we now have

$$K = H - \mu N$$

$$\psi\left(\mathbf{r},t\right) \equiv e^{itK}\psi_S\left(\mathbf{r}\right)e^{-itK} \tag{3.107}$$

$$\psi^\dagger\left(\mathbf{r},t\right) \equiv e^{itK}\psi_S^+\left(\mathbf{r}\right)e^{-itK} \tag{3.108}$$

We now proceed by analogy with the response functions. On the left we show the definitions for response functions, and on the right the analogous definitions for response functions. Let

$$G^R\left(\mathbf{r}, \mathbf{r}';t\right) = -iA\left(\mathbf{r}, \mathbf{r}';t\right)\theta\left(t\right) \quad ; \quad \chi_{ij}^R\left(t\right) = 2i\chi_{ij}''\left(t\right)\theta\left(t\right) \tag{3.109}$$

where the *spectral weight* is defined by

$$\boxed{A\left(\mathbf{r}, \mathbf{r}';t\right) \equiv \left\langle\left\{\psi\left(\mathbf{r},t\right), \psi^+\left(\mathbf{r}',0\right)\right\}\right\rangle} \quad ; \quad \chi_{ij}''\left(t\right) = \left\langle\left[A_i\left(\mathbf{r},t\right), A_j\left(\mathbf{r}',0\right)\right]\right\rangle \tag{3.110}$$

Then taking the Fourier transform, one obtains the spectral representation

$$\boxed{G^R\left(\mathbf{r}, \mathbf{r}';\omega\right) = \int_{-\infty}^\infty \frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r}, \mathbf{r}';\omega'\right)}{\omega+i\eta-\omega'}} \quad ; \quad \chi_{ij}^R\left(\omega\right) = \int_{-\infty}^\infty \frac{d\omega'}{\pi}\frac{\chi_{ij}''\left(\omega'\right)}{\omega'-\left(\omega+i\eta\right)}. \tag{3.111}$$

The spectral weight will obey sum-rules, like χ'' did. For example

$$\boxed{\int_{-\infty}^\infty \frac{d\omega'}{2\pi}A\left(\mathbf{r}, \mathbf{r}';\omega'\right) = \left\langle\left\{\psi\left(\mathbf{r},0\right), \psi^+\left(\mathbf{r}',0\right)\right\}\right\rangle = \delta\left(\mathbf{r}-\mathbf{r}'\right)} \tag{3.112}$$

From such sum rules, a high-frequency expansion can easily be found as usual. But that is not our subject for now.

To establish the relation between the Matsubara Green's function and the retarded one, and by the same token establish the spectral representation for $\mathcal{G}$, consider

$$\mathcal{G}\left(\mathbf{r}, \mathbf{r}';\tau\right) = -\left\langle\psi\left(\mathbf{r},\tau\right)\psi^+\left(\mathbf{r}',0\right)\right\rangle\theta\left(\tau\right) + \left\langle\psi^+\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},\tau\right)\right\rangle\theta\left(-\tau\right) \tag{3.113}$$

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) \tag{3.114}$$

$$= \int_0^\beta d\tau e^{ik_n\tau}\left[-\left\langle\psi\left(\mathbf{r},\tau\right)\psi^+\left(\mathbf{r}',0\right)\right\rangle\right] \tag{3.115}$$

Assume that $k_n > 0$. Then, as illustrated in Fig.(3-4), we can deform the contour of integration within the domain of analyticity along $\mathrm{Re}\left(t\right) = \mathrm{Im}\left(\tau\right) > 0$. (The analyticity of $\left\langle\psi\left(\mathbf{r},\tau\right)\psi^+\left(\mathbf{r}',0\right)\right\rangle$ in that domain comes from $e^{-\beta H}$ in the trace. You will be able to prove this later by calculating $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ with the help of the spectral representation Eq.(3.122) and tricks for evaluating sums on Matsubara frequencies). For $\mathrm{Im}\left(\tau\right) = \infty$ there will be no contribution from the small segment since $e^{ik_n\tau}$ becomes a decaying exponential. The integral becomes
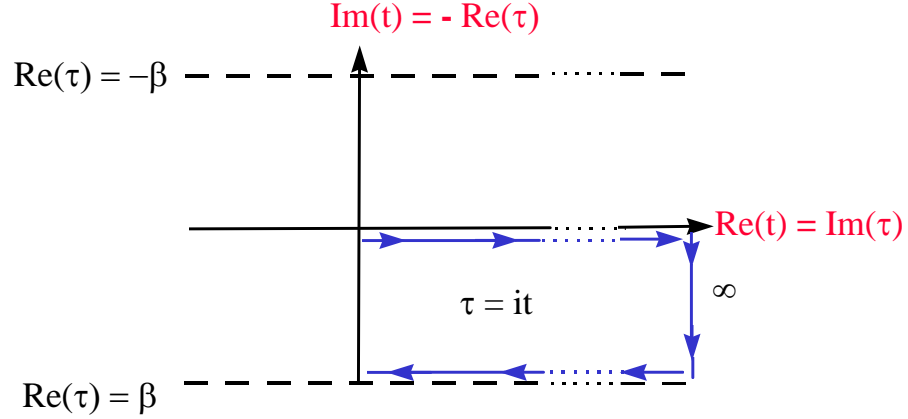
Figure 3-4   Deformed contour used to relate the Matsubara and the retarded Green's functions.

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \tag{3.116}$$

$$\int_{t=0}^{t=\infty} d\left(it\right)\left[-\left\langle e^{iKt}\psi_S\left(\mathbf{r}\right)e^{-iKt}\psi_S^+\left(\mathbf{r}'\right)\right\rangle\right]e^{ik_n\left(it\right)}$$

$$+\int_{t=\infty}^{t=0} d\left(it\right)\left[-\left\langle e^{iK\left(t-i\beta\right)}\psi_S\left(\mathbf{r}\right)e^{-iK\left(t-i\beta\right)}\psi_S^+\left(\mathbf{r}'\right)\right\rangle\right]e^{\left(ik_n\right)i\left(t-i\beta\right)}$$

In the last integral, we then use the results

$$e^{\left(ik_n\right)i\left(-i\beta\right)} = e^{\left(ik_n\right)\beta} = -1 \tag{3.117}$$

$$\int_\infty^0 = -\int_0^\infty \tag{3.118}$$

$$\left[-\left\langle e^{iK\left(t-i\beta\right)}\psi_S\left(\mathbf{r}\right)e^{-iK\left(t-i\beta\right)}\psi_S^\dagger\left(\mathbf{r}'\right)\right\rangle\right] = \left[-\left\langle e^{\beta K}e^{iKt}\psi_S\left(\mathbf{r}\right)e^{-iKt}e^{-\beta K}\psi_S^\dagger\left(\mathbf{r}'\right)\right\rangle\right] \tag{3.119}$$

It then suffices to cancel the left most $e^{\beta K}$ with the density matrix and to use the cyclic property of the trace to obtain for the integrand of the last integral,

$$= \left[-\left\langle\psi^\dagger\left(\mathbf{r}',0\right)\psi\left(\mathbf{r},t\right)\right\rangle\right]. \tag{3.120}$$

Overall then, the integral in Eq.(3.116) is equal to

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = -i\int_0^\infty dt\left\langle\left\{\psi\left(\mathbf{r},t\right),\psi^\dagger\left(\mathbf{r}',0\right)\right\}\right\rangle e^{i\left(ik_n\right)t} \tag{3.121}$$

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n-\omega'}} \tag{3.122}$$

All that we assumed to deform the contour was that $k_n > 0$. Thus, $ik_n \to \omega + i\eta$ with $\eta > 0$ is consistent with the hypothesis and allows us to deform the contour as advertized. Comparing the formula for $\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)$ for $k_n > 0$ with the expression for the retarded Green's function(3.111), we see that analytic continuation is possible.

$$\boxed{G^R\left(\mathbf{r},\mathbf{r}';\omega\right)=\lim_{ik_n\to\omega+i\eta}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)} \tag{3.123}$$

If we had started with $k_n < 0$, analytic continuation $ik_n \to \omega - i\eta$ to the advanced Green's function would have been possible.

Remark 33 *Connectedness and periodicity: For a general correlation function, similar spectral representations can also be defined for connected functions (see below) so that periodicity or anti-periodicity can be defined.*

3.4.4 Spectral weight and rules for analytical continuation

In this section, we summarize what we have learned for the analytic properties of the Matsubara Green's function and we clarify the rules for analytic continuation.[12]

The key result for understanding the analytical properties of $\mathcal{G}$ is the spectral representation Eq.(3.122)

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n-\omega'} \tag{3.124}$$

The spectral weight $A\left(\mathbf{r},\mathbf{r}';\omega'\right)$ was discussed just in the previous subsection (See also Eq.(3.179)).

The Matsubara Green's function and the retarded functions are special case of a more general function defined in the complex frequency plane by

$$\boxed{G\left(\mathbf{r},\mathbf{r}';z\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{z-\omega'}} \tag{3.125}$$

This function is analytic everywhere except on the real axis. Physically interesting special cases are

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=G\left(\mathbf{r},\mathbf{r}';ik_n\right)$$

$$G^R\left(\mathbf{r},\mathbf{r}';\omega\right)=\lim_{\eta\to 0}G\left(\mathbf{r},\mathbf{r}';\omega+i\eta\right) \tag{3.126}$$

$$G^A\left(\mathbf{r},\mathbf{r}';\omega\right)=\lim_{\eta\to 0}G\left(\mathbf{r},\mathbf{r}';\omega-i\eta\right) \tag{3.127}$$

The function $G\left(\mathbf{r},\mathbf{r}';z\right)$ has a jump on the real axis given by

$$\boxed{A\left(\mathbf{r},\mathbf{r}';\omega'\right)=i\lim_{\eta\to 0}\left[G\left(\mathbf{r},\mathbf{r}';\omega+i\eta\right)-G\left(\mathbf{r},\mathbf{r}';\omega-i\eta\right)\right]} \tag{3.128}$$

$$A\left(\mathbf{r},\mathbf{r}';\omega'\right)=i\left[G^R\left(\mathbf{r},\mathbf{r}';\omega\right)-G^A\left(\mathbf{r},\mathbf{r}';\omega\right)\right]$$

In the special case where $A\left(\mathbf{r},\mathbf{r}';\omega'\right)$ is real (which is almost always the case in practice since we consider $\mathbf{r}=\mathbf{r}'$ or $\mathbf{k}=\mathbf{k}'$), we have

$$A\left(\mathbf{r},\mathbf{r}';\omega'\right)=-2\operatorname{Im}G^R\left(\mathbf{r},\mathbf{r}';\omega\right) \tag{3.129}$$

like we have often used in the one-body case.

The previous results are summarized in Fig.(3-5) which displays the analytic structure of $G\left(\mathbf{r},\mathbf{r}';z\right)$. This function is analytical everywhere except on the real axis where it has a branch cut leading to a jump Eq.(3.128) in the value of the function as we approach the real axis from either the upper or lower complex half-plane. The limit as we come from the upper half-plane is equal to $G^R\left(\mathbf{r},\mathbf{r}';\omega\right)$ whereas from the lower half-plane it is equal to $G^A\left(\mathbf{r},\mathbf{r}';\omega\right)$. The Matsubara Green's function is defined only on a discrete but infinite set of points along the imaginary frequency axis.
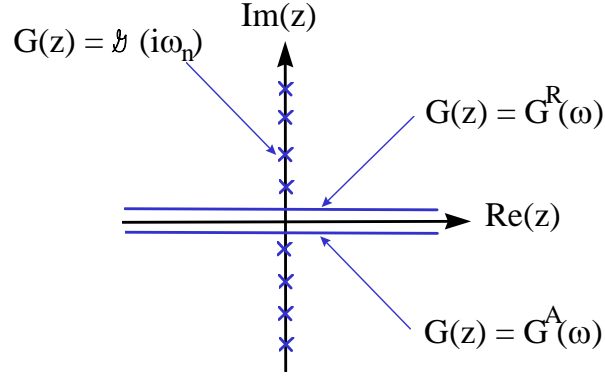

Figure 3-5   Analytical structure of $G(z)$ in the complex frequency plane. $G(z)$ reduces to either $G^R\left(\omega\right)$, $G^A\left(\omega\right)$ or $\mathcal{G}\left(i\omega_n\right)$ depending on the value of the complex frequency z. There is a branch cut along the real axis.

The problem of finding $G^R\left(\mathbf{r},\mathbf{r}';\omega\right)$ along the real-time axis from the knowledge of the Matsubara Green's function is a problem of analytical continuation. Unfortunately, $G\left(z=ik_n\right)$ does not have a unique analytical continuation because there is an infinite number of analytical functions that have the same value along this discrete set of points. For example, suppose we know $G\left(z=ik_n\right)$, then $G\left(z\right)\left(1+\left(e^{\beta z}+1\right)\right)$ has the same value as $G\left(z\right)$ for all points $z=ik_n$ because $e^{ik_n\beta}+1=0$. Baym and Mermin[13], using results from the theory of complex functions, have obtained the following result.

Theorem 8 *If*

1. $G\left(z\right)$ is analytical in the upper half-plane

2. $G\left(z\right)=\mathcal{G}\left(ik_n\right)$ for all Matsubara frequencies

3. $\lim_{z\to\infty}zG\left(z\right)=cst$

then the analytical continuation is unique and

$$G^R\left(\mathbf{r},\mathbf{r}';\omega\right)=\lim_{ik_n\to\omega+i\eta}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) \tag{3.130}$$

The key point is the third one on the asymptotic behavior at high frequency. That this is the correct asymptotic behavior at high frequency follows trivially from the spectral representation Eq.(3.125) as long as we remember that the spectral weight is bounded in frequency. The non-trivial statement is that this asymptotic behavior suffices to make the analytical continuation unique. In practice this rarely poses a problem. The simple replacement $ik_n\to\omega+i\eta$ suffices. Nevertheless, the asymptotic behavior reflects a very fundamental property of the physical system, namely the anticommutation relations! It is thus crucial to check that it is satisfied. More on the meaning of the asymptotic behavior in subsection (3.6.1).

3.4.5 Matsubara Green's function in momentum space and non-interacting case

We first present the definition of the Matsubara Green's function in momentum space since this is where, in translationally invariant systems, it will be diagonal. With our definition of momentum and real space second quantized operators, and our normalization for momentum eigenstates Eq.(**??**) we have

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right) = -\left\langle T_\tau \psi\left(\mathbf{r},\tau\right)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle = -\left\langle T_\tau \sum_{\mathbf{k}} \left\langle \mathbf{r} \left| \mathbf{k}\right\rangle c_{\mathbf{k}}\left(\tau\right) \sum_{\mathbf{k}'} c^\dagger_{\mathbf{k}'}\left(\tau'\right)\left\langle \mathbf{k}' \left| \mathbf{r}'\right\rangle \right\rangle \right.$$
(3.131)

$$\left\langle \mathbf{r} \left| \mathbf{k}\right\rangle \left\langle \mathbf{k}' \left| \mathbf{r}'\right\rangle = \frac{1}{\mathcal{V}} e^{i\mathbf{k}\cdot\mathbf{r}-i\mathbf{k}'\cdot\mathbf{r}'} = \frac{1}{\mathcal{V}} e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)+i\left(\frac{\mathbf{k}+\mathbf{k}'}{2}\right)\cdot\left(\mathbf{r}-\mathbf{r}'\right)}.$$
(3.132)

Assuming space translation invariance, we can integrate over the center of mass coordinate $\frac{1}{\mathcal{V}}\int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) = 1$. Since

$$\frac{1}{\mathcal{V}}\int d\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right) e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\left(\frac{\mathbf{r}'+\mathbf{r}}{2}\right)} = \frac{1}{\mathcal{V}}\left(2\pi\right)^3 \delta\left(\mathbf{k}-\mathbf{k}'\right) = \delta_{\mathbf{k},\mathbf{k}'}$$
(3.133)

we are left with

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\tau'\right) = -\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}\left(\tau\right) c^\dagger_{\mathbf{k}'}\left(\tau'\right) e^{i\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\right\rangle$$
(3.134)

$$\mathcal{G}\left(\mathbf{k};\tau-\tau'\right) = \int d\left(\mathbf{r}-\mathbf{r}'\right) e^{-i\mathbf{k}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\left[-\left\langle T_\tau \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'} c_{\mathbf{k}'}\left(\tau\right) c^\dagger_{\mathbf{k}'}\left(\tau'\right) e^{i\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\right\rangle\right]$$
(3.135)

$$\boxed{\mathcal{G}\left(\mathbf{k};\tau-\tau'\right) = -\left\langle T_\tau c_{\mathbf{k}}\left(\tau\right) c^\dagger_{\mathbf{k}}\left(\tau'\right)\right\rangle}$$
(3.136)

which could have been guessed from the start! Our definitions of Fourier transforms just make this work.

Remark 34 *Momentum indices and translational invariance: Note that the conservation of total momentum corresponding to translational invariance corresponds to the sum of the momentum indices of the creation-annihilation operators being equal to zero. The sign of momentum is counted as negative when it appears on a creation operator.*

Example of non-interacting particles

For non-interacting particles let us consider a quadratic diagonal Hamiltonian

$$K_0 = \sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} - \mu\right) c^+_{\mathbf{k}} c_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c^+_{\mathbf{k}} c_{\mathbf{k}}$$
(3.137)

The result for the Green's function may be obtained either directly from the definition or by integrating the equations of motion. Both ways of obtaining the simple result

$$\boxed{\mathcal{G}_0\left(\mathbf{k};ik_n\right) = \frac{1}{ik_n-\zeta_{\mathbf{k}}}}$$
(3.138)

are instructive, so let us do both. Assuming for one moment that the above result is correct, our rules for analytic continuation then immediately give us the retarded function

$$\boxed{G^R\left(\mathbf{k};\omega\right) = \frac{1}{\omega+i\eta-\zeta_{\mathbf{k}}}}$$
(3.139)

that has precisely the form we expect from our experience with the one-body case. The only difference with the one-body case is in the presence of the chemical potential in $\zeta_{\mathbf{k}}$.

From the definition To evaluate the Green's function from its definition, we need $c_{\mathbf{k}}(\tau)$. That quantity may be obtained by solving the Heisenberg equations of motion,

$$\frac{\partial c_{\mathbf{k}}}{\partial \tau} = [K_0, c_{\mathbf{k}}] = -\zeta_{\mathbf{k}} c_{\mathbf{k}} \tag{3.140}$$

The anticommutator was easy to evaluate using our standard trick Eq.(3.9). The resulting differential equation is easy to integrate given the initial condition on Heisenberg operators. We obtain,

$$c_{\mathbf{k}}(\tau) = e^{-\zeta_{\mathbf{k}}\tau} c_{\mathbf{k}} \tag{3.141}$$

so that substituting in the definition,

$$\mathcal{G}_0(\mathbf{k};\tau) = -\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^+ \right\rangle = -e^{-\zeta_{\mathbf{k}}\tau}\left[\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \right\rangle \theta(\tau) - \left\langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \right\rangle \theta(-\tau)\right] \tag{3.142}$$

using the standard result from elementary statistical mechanics,

$$\left\langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \right\rangle = f(\zeta_{\mathbf{k}}) = \frac{1}{e^{\beta\zeta_{\mathbf{k}}} + 1} \tag{3.143}$$

and $\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \right\rangle = 1 - \left\langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \right\rangle$ we obtain

$$\boxed{\mathcal{G}_0(\mathbf{k};\tau) = -e^{-\zeta_{\mathbf{k}}\tau}\left[(1 - f(\zeta_{\mathbf{k}}))\theta(\tau) - f(\zeta_{\mathbf{k}})\theta(-\tau)\right]} \tag{3.144}$$

Remark 35 *Inadequacy of Matsubara representation outside the domain of definition: We see here clearly that if $\tau < 0$ the equality*

$$\mathcal{G}_0(\mathbf{k};\tau + \beta) = -\mathcal{G}_0(\mathbf{k};\tau) \tag{3.145}$$

is satisfied because $e^{-\zeta_{\mathbf{k}}\beta}(1 - f(\zeta_{\mathbf{k}})) = f(\zeta_{\mathbf{k}})$. On the other hand,

$$\mathcal{G}_0(\mathbf{k};\tau + 3\beta) \neq \mathcal{G}_0(\mathbf{k};\tau + \beta) \tag{3.146}$$

as we might have believed if we had trusted the expansion

$$\mathcal{G}_0(\mathbf{k};\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-ik_n\tau}\mathcal{G}_0(\mathbf{k};ik_n)$$

outside its domain of validity! The conclusion is that as long as the Matsubara frequency representation is used to compute functions inside the domain $-\beta < \tau < \beta$, it is correct. The perturbation expansion of the interaction picture does not force us to use Green's functions outside this domain, so the Matsubara representation is safe!

Remark 36 *Alternate evaluation of time evolution: We could have obtained the time evolution also by using the identity*

$$e^A C e^A = C + [A, C] + \frac{1}{2!}[A, [A, C]] + \frac{1}{3!}[A, [A, [A, C]]] + \ldots \tag{3.147}$$

that follows from expanding the exponential operators. This is less direct.

Remark 37 *Appearance of $\mathcal{G}_0(\mathbf{k};\tau)$: It is instructive to plot $\mathcal{G}_0(\mathbf{k};\tau)$ as a function of imaginary time. In some energy units, let us take $\beta = 5$, and then consider three possible values of $\zeta_{\mathbf{k}}$. First $\zeta_{\mathbf{k}} = 0.2$, i.e. for a value of momentum above the Fermi surface, then a value right at the Fermi surface, $\zeta_{\mathbf{k}} = 0$ and finally a value $\zeta_{\mathbf{k}} = -0.2$ corresponding to a momentum right below the Fermi surface. These cases are illustrated respectively in Figs.(3-6) to (3-8). Note that the jump at $\tau = 0$ is always unity, reflecting the anticommutation relations. What is meant by antiperiodicity also becomes clear. The extremal values near $\pm\beta$ and ± 0 are simply related to the occupation number, independently of interactions.*
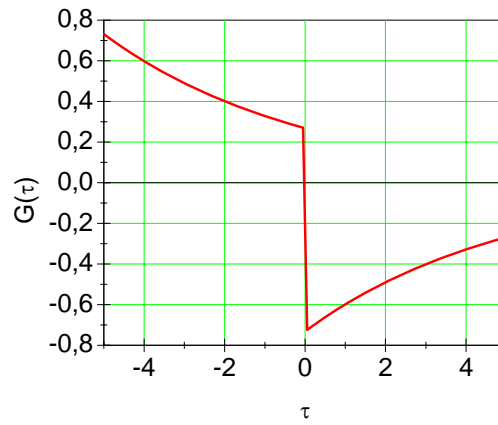
Figure 3-6 $\mathcal{G}_0\left(\mathbf{p}, \tau\right)$ for a value of momentum above the Fermi surface.
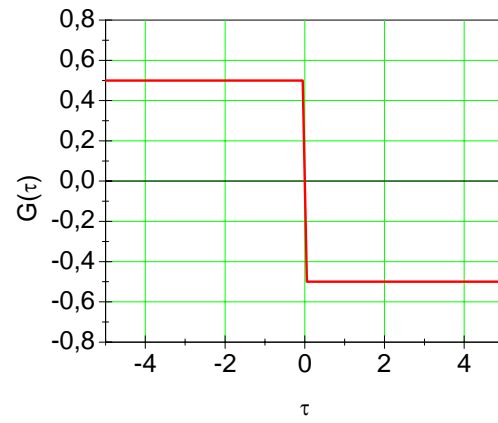

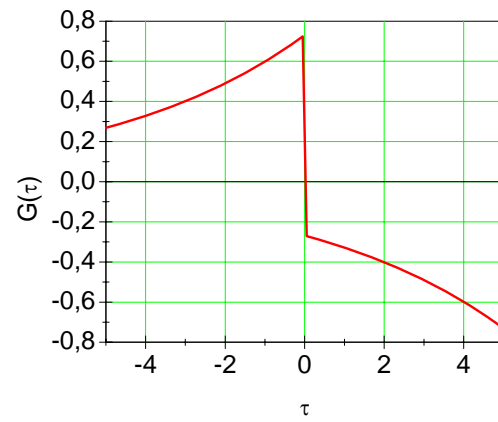Figure 3-7 $\mathcal{G}_0\left(\mathbf{p}, \tau\right)$ for a value of momentum at the Fermi surface.

Figure 3-8 $\mathcal{G}_0\left(\mathbf{p}, \tau\right)$ for a value of momentum below the Fermi surface.

GREEN FUNCTIONS

Let us continue with the derivation of the Matsubara frequency result $\mathcal{G}_0(\mathbf{k}; ik_n)$.

$$\mathcal{G}_0(\mathbf{k}; ik_n) = \int_0^\beta d\tau e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau) = -\left(1 - f(\zeta_\mathbf{k})\right) \int_0^\beta d\tau e^{ik_n\tau} e^{-\zeta_\mathbf{k}\tau} \quad (3.148)$$

$$= -\left(1 - f(\zeta_\mathbf{k})\right) \frac{e^{ik_n\beta} e^{-\zeta_\mathbf{k}\beta} - 1}{ik_n - \zeta_\mathbf{k}} \quad (3.149)$$

$$= -\left(1 - f(\zeta_\mathbf{k})\right) \frac{-e^{-\zeta_\mathbf{k}\beta} - 1}{ik_n - \zeta_\mathbf{k}} = \frac{1}{ik_n - \zeta_\mathbf{k}} \quad (3.150)$$

The last equality follows because

$$\left(1 - f(\zeta_\mathbf{k})\right) = \frac{e^{\zeta_\mathbf{k}\beta}}{e^{\zeta_\mathbf{k}\beta} + 1} = \frac{1}{e^{-\zeta_\mathbf{k}\beta} + 1} \quad (3.151)$$

We thus have our final result Eq.(3.138) for non-interacting particles.

From the equations of motion   In complete analogy with the derivation in subsection (3.1.1) we can obtain the equations of motion in the quadratic case.

$$\frac{\partial}{\partial \tau} \mathcal{G}_0(\mathbf{k}; \tau) = -\frac{\partial}{\partial \tau} \left\langle T_\tau c_\mathbf{k}(\tau) c_\mathbf{k}^\dagger \right\rangle \quad (3.152)$$

$$= -\delta(\tau) \left\langle \left\{ c_\mathbf{k}(\tau), c_\mathbf{k}^\dagger \right\} \right\rangle - \left\langle T_\tau \left(\frac{\partial}{\partial \tau} c_\mathbf{k}(\tau) \right) c_\mathbf{k}^\dagger \right\rangle \quad (3.153)$$

Using the equal-time anticommutation relations as well as the Heisenberg equations of motion for free particles Eq.(3.140) the above equation becomes,

$$\frac{\partial}{\partial \tau} \mathcal{G}_0(\mathbf{k}; \tau) = -\delta(\tau) + \zeta_\mathbf{k} \left\langle T_\tau c_\mathbf{k}(\tau) c_\mathbf{k}^\dagger \right\rangle \quad (3.154)$$

so that the equation of motion for the Matsubara propagator is

$$\boxed{\left(\frac{\partial}{\partial \tau} + \zeta_\mathbf{k} \right) \mathcal{G}_0(\mathbf{k}; \tau) = -\delta(\tau)} \quad (3.155)$$

To obtain the Matsubara-frequency result, we only need to integrate on both sides using the general expression to obtain Fourier coefficients Eq.(3.105)

$$\int_{0^-}^{\beta^-} \left[\left(\frac{\partial}{\partial \tau} + \zeta_\mathbf{k} \right) \mathcal{G}_0(\mathbf{k}; \tau) \right] e^{ik_n\tau} d\tau = -1 \quad (3.156)$$

so that integrating by parts,

$$e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau)|_{0^-}^{\beta^-} - ik_n \mathcal{G}_0(\mathbf{k}; ik_n) + \zeta_\mathbf{k} \mathcal{G}_0(\mathbf{k}; ik_n) = -1 \quad (3.157)$$

Note that we had to specify that the domain of integration includes 0. The integrated term disappears because of the KMS boundary conditions (antiperiodicity) Eq.(3.94). Indeed, antiperiodicity implies that

$$e^{ik_n\tau} \mathcal{G}_0(\mathbf{k}; \tau)|_{0^-}^{\beta^-} = -\mathcal{G}_0(\mathbf{k}; \beta^-) - \mathcal{G}_0(\mathbf{k}; 0^-) = 0 \quad (3.158)$$

Eq.(3.157) for the Matsubara Green's function then immediately gives us the desired result Eq.(3.138).

3.4.6 Sums over Matsubara frequencies

In doing practical calculations, we will have to become familiar with sums over Matsubara frequencies. When we have products of Green's functions, we will use partial fractions in such a way that we will basically always have to evaluate sums such as

$$T \sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{3.159}$$

where $T = \beta^{-1}$. We have however to be careful since the result of this sum is ambiguous. Indeed, returning back to the motivation for these sums, recall that

$$\mathcal{G}(\mathbf{k};\tau) = T \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} \tag{3.160}$$

We already know that the Green's function has a jump at $\tau = 0$. In other words,

$$\left[\lim_{\tau \to 0^+} \mathcal{G}(\mathbf{k};\tau) = -\langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \rangle \right] \neq \left[\lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k};\tau) = \langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \rangle \right] \tag{3.161}$$

This inequality in turn means that

$$T \sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} \neq T \sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} \neq T \sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{3.162}$$

The sum does not converge uniformly in the interval including $\tau = 0$ because the $1/n$ decrease for $n \to \infty$ is too slow. Even if we can obtain a finite limit for the last sum by combining positive and negative Matsubara frequencies, what makes physical sense is only one or the other of the two limits $\tau \to 0^{\pm}$.

Remark 38 Remark 39 *The jump*, $\lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k};\tau) - \lim_{\tau \to 0^+} \mathcal{G}(\mathbf{k};\tau)$ *is always equal to unity because of the anticommutation relations. The slow convergence in* $1/ik_n$ *is thus a reflection of the anticommutation relations and will remain true even in the interacting case. If the* $(ik_n)^{-1}$ *has a coefficient different from unity, the spectral weight is not normalized and the jump is not unity. This will be discussed shortly.*

Let us evaluate the Matsubara frequency sums. Considering again the case of fermions we will show as special cases that

$$\boxed{T \sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} = \frac{1}{e^{\beta \zeta_{\mathbf{k}}} + 1} = f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k};0^-)} \tag{3.163}$$

$$\boxed{T \sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} = \frac{-1}{e^{-\beta \zeta_{\mathbf{k}}} + 1} = -1 + f(\zeta_{\mathbf{k}}) = \mathcal{G}_0(\mathbf{k};0^+)} \tag{3.164}$$

Obviously, the non-interacting Green's function has the correct jump $\mathcal{G}_0(\mathbf{k};0^-) - \mathcal{G}_0(\mathbf{k};0^+) = 1$

Proof: [14]To perform the sum over Matsubara frequencies, the standard trick is to go to the complex plane. The following function

$$-\beta \frac{1}{e^{\beta z} + 1} \tag{3.165}$$

has poles for z equal to any fermionic Matsubara frequency: $z = ik_n$. Its residue at these poles is unity since for

$$z = ik_n + \delta z \tag{3.166}$$

we have

$$-\beta \frac{1}{e^{\beta z}+1} = -\beta \frac{1}{e^{ik_n\beta+\beta\delta z}+1} = -\beta \frac{1}{-1e^{\beta\delta z}+1} \tag{3.167}$$

$$\lim_{z-ik_n\to 0} \delta z \left[-\beta \frac{1}{e^{\beta z}+1} \right] = 1 \tag{3.168}$$

Similarly the following function has the same poles and residues:

$$\lim_{z-ik_n\to 0} \delta z \left[\beta \frac{1}{e^{-\beta z}+1} \right] = 1 \tag{3.169}$$

To evaluate the $\tau < 0$ case by contour integration, we use Cauchy's theorem on the contour C_1, which is a sum of circles going counterclockwise around the points where z is equal to the Matsubara frequencies. Using Eq.(3.168) this allows us to establish the equality

$$\frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = -\frac{1}{2\pi i} \int_{C_1} \frac{dz}{e^{\beta z}+1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \tag{3.170}$$

This contour can be deformed, as illustrated in Fig.(3-9), into $C_2 + C_3$ (going through C_1') with no contribution from the semi-circles at $\mathrm{Re}\,(z) = \pm\infty$ because $\frac{1}{e^{\beta z}+1}$ insures convergence when $\mathrm{Re}\,(z) > 0$ despite $e^{-z\tau}$ in the numerator, and $e^{-z\tau}$ insures convergence when $\mathrm{Re}\,(z) < 0$, $\tau < 0$. With the deformed contour $C_2 + C_3$, only the contribution from the pole in the clockwise direction is left so that we have

$$\boxed{\frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = \frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{\beta\zeta_{\mathbf{k}}}+1} = e^{-\zeta_{\mathbf{k}}\tau} f(\zeta_{\mathbf{k}})} \tag{3.171}$$

which agrees with the value of $\mathcal{G}_0(\mathbf{k};\tau)$ in Eq.(3.144) when $\tau < 0$. In particular, when $\tau = 0^-$ we have proven the identity (3.164) . To evaluate the

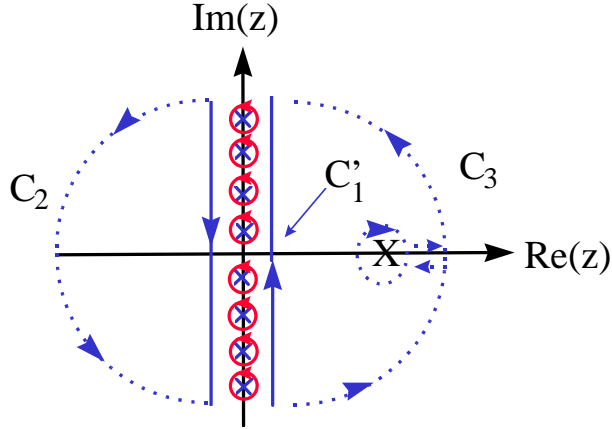Figure 3-9   Evaluation of fermionic Matsubara frequency sums in the complex plane.

$\tau > 0$ case we use the same contour but with the other form of auxiliary function Eq.(3.169). We then obtain,

$$\frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{C_1} \frac{dz}{e^{-\beta z}+1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \tag{3.172}$$

This contour can be deformed into $C_2 + C_3$ with no contribution from the semi-circles at $\mathrm{Re}\,(z) = \pm\infty$ because this time $e^{-z\tau}$ insures convergence when $\mathrm{Re}\,(z) > 0$, $\tau > 0$ and $\frac{1}{e^{-\beta z}+1}$ ensures convergence when $\mathrm{Re}\,(z) < 0$ despite $e^{-z\tau}$ in the numerator. Again, from $C_2 + C_3$, only the contribution from the pole in the clockwise direction survives so that we have

$$\boxed{\frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -\frac{e^{-\zeta_{\mathbf{k}}\tau}e^{\beta\zeta_{\mathbf{k}}}}{e^{\beta\zeta_{\mathbf{k}}}+1} = -e^{-\zeta_{\mathbf{k}}\tau}\left(1 - f\left(\zeta_{\mathbf{k}}\right)\right)} \quad (3.173)$$

which agrees with the value of $\mathcal{G}_0\left(\mathbf{k}; \tau\right)$ in Eq.(3.144) when $\tau < 0$. In particular, when $\tau = 0^+$ we have proven the identity (3.163).

3.5 Physical meaning of the spectral weight: Quasiparticles, effective mass, wave function renormalization, momentum distribution.

To discuss the Physical meaning of the spectral weight, we first find it in the non-interacting case, then write a formal general expression, the Lehman representation, that allows us to see its more general meaning. After our discussion of a photoemission experiment, we will be in a good position to understand the concepts of quasiparticles, wave-function renormalization, effective mass and momentum distribution. We will even have a first look at Fermi liquid theory, and see how it helps us to understand photoemission experiments.

3.5.1 Spectral weight for non-interacting particles

The general result for the spectral weight in terms of the Green's function Eq.(3.128) gives us for non-interacting particles

$$A_0\left(\mathbf{k}, \omega\right) = i\left[\frac{1}{\omega + i\eta - \zeta_{\mathbf{k}}} - \frac{1}{\omega - i\eta - \zeta_{\mathbf{k}}}\right] \quad (3.174)$$

$$= 2\pi\delta\left(\omega - \zeta_{\mathbf{k}}\right) \quad (3.175)$$

In physical terms, this tells us that for non-interacting particles in a translationally invariant system, a single excited particle or hole of momentum $\mathbf{k}$ added to an eigenstate is an true excited eigenstate located an energy $\omega = \zeta_{\mathbf{k}}$ above or below the Fermi level. In the interacting case, the Lehman representation will show us clearly that what we just said is the correct interpretation

3.5.2 Lehman representation

For a general correlation function, not necessarily a Green's function, one establishes the connection between Matsubara functions and retarded functions by using the Lehman representation. This representation is also extremely useful to extract

the physical significance of the poles of correlation functions so this is why we introduce it at this point. We have already seen examples of Lehman representation in the one-body case when we wrote in Eq.(3.30),

$$G^R\left(\mathbf{r},\mathbf{r}';\omega\right) = \sum_n \frac{\phi_n\left(\mathbf{r}\right)\phi_n^*\left(\mathbf{r}'\right)}{\omega + i\eta - E_n}$$

Let us consider the more general many-body case, starting from the Matsubara Green's function. It suffices to insert a complete set of energy eigenstates between each field operator in the expression for the spectral weight

$$
\begin{aligned}
A\left(\mathbf{r},\mathbf{r}';t\right) &\equiv \left\langle \left\{ \psi\left(\mathbf{r},t\right),\psi^+\left(\mathbf{r}',0\right)\right\}\right\rangle \qquad\qquad (3.176)\\
&= e^{\beta\Omega}\sum_{m,n}\left[\langle n|\,e^{-\beta K}e^{iKt}\psi_S\left(\mathbf{r}\right)e^{-iKt}\,|m\rangle\,\langle m|\,\psi_S^\dagger\left(\mathbf{r}'\right)|n\rangle\right.\\
&\qquad\qquad \left.+\,\langle n|\,e^{-\beta K}\psi_S^\dagger\left(\mathbf{r}'\right)|m\rangle\,\langle m|\,e^{iKt}\psi_S\left(\mathbf{r}\right)e^{-iKt}\,|n\rangle\right]
\end{aligned}
$$

We now use $e^{-iKt}\,|n\rangle = e^{-iK_n t}\,|n\rangle$ with $K_n = E_n - \mu N_n$ if there are N_n particles in the initial state $|n\rangle$. In the first term above, $\langle n|$ has one less particle than $|m\rangle$ while the reverse is true in the second term so that $K_m - K_n = \left(E_m - \mu\left(N_n + 1\right) - E_n + \mu N_n\right)$ in the first term and $K_n - K_m = \left(E_n - \mu N_n - E_m + \mu\left(N_n - 1\right)\right)$ in the second. Taking the Fourier transform $\int dt e^{i\omega' t}$ we have

$$
\begin{aligned}
A\left(\mathbf{r},\mathbf{r}';\omega'\right) &= e^{\beta\Omega}\times \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.177)\\
&\quad \sum_{mn}\left[e^{-\beta K_n}\,\langle n|\,\psi_S\left(\mathbf{r}\right)|m\rangle\,\langle m|\,\psi_S^\dagger\left(\mathbf{r}'\right)|n\rangle\,2\pi\delta\left(\omega' - \left(E_m - \mu - E_n\right)\right)\right.\\
&\quad \left.+\,e^{-\beta K_n}\,\langle n|\,\psi_S^\dagger\left(\mathbf{r}'\right)|m\rangle\,\langle m|\,\psi_S\left(\mathbf{r}\right)|n\rangle\,2\pi\delta\left(\omega' - \left(E_n - \mu - E_m\right)\right)\right]
\end{aligned}
$$

One can interpret Physically the spectral weight as follows. It has two pieces, the first one for excited states with one more particle, and the second one for excited states with one more hole. Photoemission experiments (See Einstein's Nobel prize) access this last piece of the spectral weight, while Bremsstrahlung inverse spectroscopy (BIS) experiments measure the first piece.[1] Excited particle states contribute to positive frequencies ω' if their excitation energy is larger than the chemical potential, $E_m - E_n > \mu$ and to negative frequencies otherwise. Zero frequency means that the excitation energy is equal to the chemical potential. In other words, every excited single-particle or single-hole state corresponds to a delta function in the spectral weight whose weight depends on the overlap between initial states with one more particle at $\mathbf{r}'$ or one more hole at $\mathbf{r}$, and the true excited states.

Remark 40 *At zero temperature, we have*

$$
\begin{aligned}
A\left(\mathbf{r},\mathbf{r}';\omega'\right) &= Z^{-1}\sum_m\left[\langle 0|\,\psi_S\left(\mathbf{r}\right)|m\rangle\,\langle m|\,\psi_S^\dagger\left(\mathbf{r}'\right)|0\rangle\,2\pi\delta\left(\omega' - \left(E_m - \mu - E_0\right)\right)\right.\\
&\quad \left.+\,\langle 0|\,\psi_S^\dagger\left(\mathbf{r}'\right)|m\rangle\,\langle m|\,\psi_S\left(\mathbf{r}\right)|0\rangle\,2\pi\delta\left(\omega' - \left(E_0 - \mu - E_m\right)\right)\right](3.178)
\end{aligned}
$$

Since to add a particle we need at least an energy μ, then $E_m - \mu - E_0 > 0$ and the first term, that adds particles, contributes only to positive frequencies. On the other hand, if we remove a particle, $E_0 - \mu - E_m < 0$ since the thermodynamic result $\partial E/\partial N = \mu$ implies, with $dN = -1$, that $E_0 - E_m < \mu$ (the equality being satisfied only for the hole infinitesimally close to the Fermi surface) so that the second term, that adds holes, contributes only to the negative frequencies.

---

[1] To be more specific, these experiments add or remove particles in momentum, not position eigenstates. The only change that this implies in the discussion above is that $\psi_S^{(\dagger)}\left(\mathbf{r}\right)$ should be replaced by $c_{\mathbf{p}}^{(\dagger)}$.

The spectral representation Eq.(3.122) immediately tells us that the poles of the single-particle Green's functions are at the same position as delta functions in the spectral weight, in other words they are at the excited single-particle or single-hole states. Doing changes of dummy summation indices we can arrange so that it is always $\langle n|$ that has one less particle. Then,

$$\boxed{A\left(\mathbf{r},\mathbf{r}';\omega'\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n} + e^{-\beta K_m}\right)\langle n|\,\psi_S\left(\mathbf{r}\right)|m\rangle\,\langle m|\,\psi_S^\dagger\left(\mathbf{r}'\right)|n\rangle\,2\pi\delta\left(\omega' - \left(K_m - K_n\right)\right)}$$

$$(3.179)$$

Substituting in the spectral representation Eq.(3.122) we have,

$$\boxed{\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m} + e^{-\beta K_n}\right)\frac{\langle n|\psi_S(\mathbf{r})|m\rangle\langle m|\psi_S^\dagger(\mathbf{r}')|n\rangle}{ik_n - (E_m - E_n - \mu)}}$$

$$(3.180)$$

This is the Lehman representation. It tells us how to interpret the poles of the analytically continued $\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right).$

Remark 41 *Standard way of proving analytical continuation formula: The standard way of proving that $G^R\left(\omega\right) = \lim_{ik_n\to\omega+i\eta}\mathcal{G}\left(ik_n\right)$ is to first find the Lehman representation for both quantities.*

3.5.3 Probabilistic interpretation of the spectral weight

For a different representation, for example for momentum, we have [15] in the translationally invariant case, by analogy with the above result for the spectral weight Eq.(3.179)

$$\boxed{A\left(\mathbf{k},\omega'\right) = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_m} + e^{-\beta K_n}\right)|\langle n|\,c_\mathbf{k}\,|m\rangle|^2\,2\pi\delta\left(\omega' - \left(K_m - K_n\right)\right).}$$

$$(3.181)$$

The overlap matrix element $|\langle n|\,c_\mathbf{k}\,|m\rangle|^2$ that gives the magnitude of the delta function contribution to the spectral weight represents the overlap between the initial state with one more particle or hole in a momentum eigenstate and the true excited one-particle or one-hole state. The last equation clearly shows that $A\left(\mathbf{k},\omega'\right)/\left(2\pi\right)$ is positive and we already know that it is normalized to unity,

$$\int\frac{d\omega'}{2\pi}A\left(\mathbf{k},\omega'\right) = \left\langle\left\{c_\mathbf{k},c_\mathbf{k}^\dagger\right\}\right\rangle = 1.\qquad(3.182)$$

Hence it can be interpreted as the probability that a state formed from a true eigenstate $|n\rangle$ either by adding a particle in a single-particle state $\mathbf{k}$, namely $c_\mathbf{k}^\dagger\,|n\rangle$ (or adding a hole $c_\mathbf{k}\,|n\rangle$ in a single-particle state $\mathbf{k}$) is a true eigenstate whose energy is ω above or below the chemical potential. Clearly, adding a particle or a hole in a momentum eigenstate will lead to a true many-body eigenstate only if the momentum of each particle is individually conserved. This occurs only in the non-interacting case, so this is why the spectral weight is then a single delta function. In the more general case, many energy eigenstates will have a non-zero overlap with the state formed by simply adding a particle or a hole in a momentum eigenstate. While particle-like excitations will overlap mostly with eigenstates that are reached by adding positive ω, they can also overlap eigenstates that are reached by adding negative ω. In an analogous manner, hole-like eigenstates will be mostly at negative ω. Let us see how this manifests itself in a specific experiment.

Remark 42 *Energy vs momentum in an interacting system: It is clear that in an interacting system one must distinguish the momentum and the energy variables.*

The energy variable is ω. Knowing the momentum of a single added electron or hole is not enough to know the added energy. This added energy would be $k^2/2m$ only in the case of non-interacting electrons.

Remark 43 *Physical reason for high-frequency fall-off: The explicit expression for the spectral weight Eq.(3.181) suggests why the spectral weight falls off fast at large frequencies for a given $\mathbf{k}$, as we have discussed in Subsection (3.6.1). A state formed by adding one particle (or one hole) of momentum $\mathbf{k}$ should have exponentially small overlap with the true eigenstates of the system that have one more particle (or hole) but an arbitrarily large energy difference ω with the initial state.*

3.5.4 Angle-resolved photoemission spectroscopy (ARPES) on a Fermi liquid compound.

In a photoemission experiment, a photon ejects an electron from a solid. This is nothing but the old familiar photoelectric effect. In the angle resolved version of this experiment (ARPES), the energy and the direction of the outgoing electron are measured. This is illustrated in Fig.(3-10). The outgoing electron energy can be measured. Because it is a free electron, this measurement gives the value of the wave vector through $k^2/2m$. Using energy conservation, the energy of the outgoing electron is equal to the energy of the incident photon E_{ph}, minus the work function W plus the energy of the electron in the system, ω, measured relative to the Fermi level.
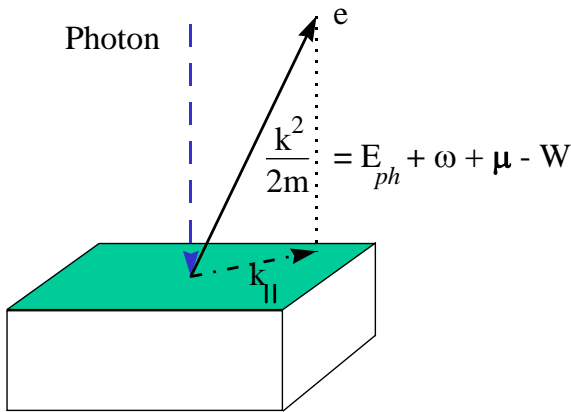
Figure 3-10   Schematic representation of an angle-resolved photoemission experiment.

The energy of the electron in the system ω will be mostly negative. The value of $\mathbf{k}_{||}$ may be extracted by simple geometric considerations from the value of k. Since in this experiment there is translational invariance only in the direction parallel to the plane, this means that in fact it is only the value of $\mathbf{k}_{||}$ that is conserved. Hence, it is only for layered systems that we really have access to both energy ω and total momentum $\mathbf{k}_{||}$ of the electron when it was in the system. Without going into details of the assumptions going into the derivation, Fermi's golden rule suggests, (see first section of Chapter 2) that the cross section for ejecting an electron of momentum $\mathbf{k}_{||}$ and energy ω (measured with respect to μ)

is proportional to

$$\frac{\partial^2 \sigma}{\partial\Omega\partial\omega} \quad \propto \quad \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega + \mu - (E_m - E_n)\right) \qquad (3.183)$$

$$\propto \quad \sum_{mn} e^{-\beta K_m} \left| \langle n| c_{\mathbf{k}_{||}} |m\rangle \right|^2 \delta\left(\omega - (K_m - K_n)\right) \qquad (3.184)$$

$$\propto \quad \int dt e^{i\omega t} \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \right\rangle \qquad (3.185)$$

which is "half" of the spectral weight (the mostly negative-energy part). More specifically, we can rewrite this result in terms of the spectral weight as follows,

$$\frac{\partial^2 \sigma}{\partial\Omega\partial\omega} \propto f(\omega) A\left(\mathbf{k}_{||}, \omega\right). \qquad (3.186)$$

Note the analogy with the cross section we found earlier for electron scattering. It was expressed in Eq.(2.1) in terms of a density-density correlation function. Through the fluctuation-dissipaton theorem Eq.(2.121), it was related to a spectral weight χ'' (analogous to A) through the Bose function (analogous to the Fermi function).

Proof: The most direct and simple proof is from the Lehman representation Eq.(3.181). To get a few more general results about $G^<\left(\mathbf{k}_{||}, \omega\right)$ and $G^>\left(\mathbf{k}_{||}, \omega\right)$ we present the following alternate proof. The cross section is proportional to the Fourier transform of $G^<\left(\mathbf{k}_{||}, \omega\right)$ as defined in Eq.(3.84).

$$\frac{\partial^2 \sigma}{\partial\Omega\partial\omega} \propto -iG^<\left(\mathbf{k}_{||}, \omega\right) \qquad (3.187)$$

One can relate $G^<$ and $G^>$ to the spectral weight in a very general way through the Fermi function. This is done using the usual cyclic property of the trace (fluctuation-dissipation theorem). From

$$\left\langle c_{\mathbf{k}_{||}}(t) c_{\mathbf{k}_{||}}^\dagger \right\rangle \quad = \quad Z^{-1}\text{Tr}\left[e^{-\beta K} \left(e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt} \right) c_{\mathbf{k}_{||}}^\dagger \right] \qquad (3.188)$$

$$= \quad Z^{-1}\text{Tr}\left[\left(e^{\beta K} e^{-\beta K} \right) c_{\mathbf{k}_{||}}^\dagger e^{-\beta K} \left(e^{iKt} c_{\mathbf{k}_{||}} e^{-iKt} \right) \right] \quad (3.189)$$

$$= \quad \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t + i\beta) \right\rangle \qquad (3.190)$$

one finds by simple use of definitions and change of integration variables,

$$A\left(\mathbf{k}_{||}, \omega\right) \quad = \quad \int dt e^{i\omega t} \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) + c_{\mathbf{k}_{||}}(t) c_{\mathbf{k}_{||}}^\dagger \right\rangle \qquad (3.191)$$

$$= \quad \int dt e^{i\omega t} \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \right\rangle + \int dt e^{i\omega(t + i\beta - i\beta)} \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t + i\beta) \right\rangle$$

$$= \quad \left(1 + e^{\beta\omega}\right) \int dt e^{i\omega t} \left\langle c_{\mathbf{k}_{||}}^\dagger c_{\mathbf{k}_{||}}(t) \right\rangle \qquad (3.192)$$

$$= \quad f(\omega)^{-1} \left(-iG^<\left(\mathbf{k}_{||}, \omega\right)\right) \qquad (3.193)$$

Substituting in Eq.(3.187) proves Eq.(3.186). Note that since

$$A\left(\mathbf{k}_{||}, \omega\right) = -i\left[G^<\left(\mathbf{k}_{||}, \omega\right) - G^>\left(\mathbf{k}_{||}, \omega\right) \right] \qquad (3.194)$$

we also have the result

$$iG^>\left(\mathbf{k}_{||}, \omega\right) = (1 - f(\omega)) A\left(\mathbf{k}_{||}, \omega\right) \qquad (3.195)$$

The theoretical formula for the photoemission cross-section Eq.(3.186) neglects processes where energy is transferred from the outgoing electron to phonons or other excitations before it is detected (multiple scattering of outgoing electron). Such processes are referred to as "inelastic background".

The state of technology and historical coincidences have conspired so that the first class of layered (quasi-two-dimensional) compounds that became available for ARPES study around 1990 were high temperature superconductors. These materials have properties that make them non-conventional materials that are not yet understood using standard approaches of solid-state Physics. Hence, people started to look for two-dimensional materials that would behave as expected from standard models. Such a material, semimetallic $TiTe_2$ was finally found around 1992. For our purposes, quasi-to-dimensional just means here that the Fermi velocity perpendicular to the planes is much smaller than the Fermi velocity in the planes. The results of this experiment[19] appear in Fig.(3-11).
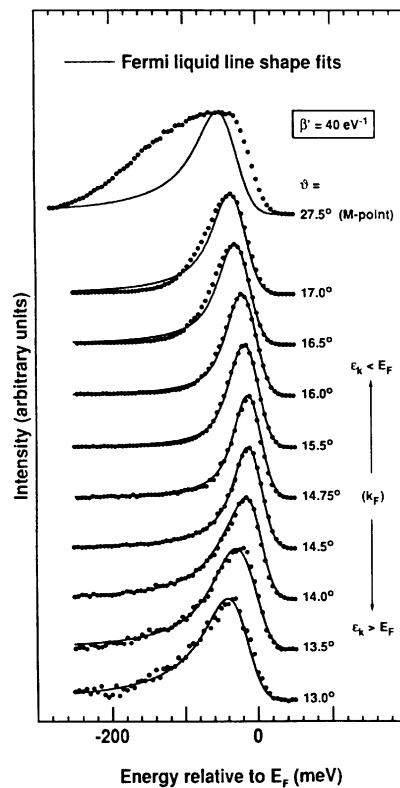
Figure 3-11   ARPES spectrum of $1 - T - TiTe_2$, after R. Claessen, R.O. Anderson, J.W. Allen, C.G. Olson, C. Janowitz, W.P. Ellis, S. Harm, M. Kalning, R. Manzke, and M. Skibowski, Phys. Rev. Lett **69**, 808 (1992).

We have to remember that the incident photon energy is $21.2 eV$ while the variation of ω is on a scale of $200 meV$ so that, for all practical purposes, the momentum vector in Fig.(3-10) is a fixed length vector. Hence, the angle with respect to the incident photon suffices to define the value of $\mathbf{k}_{||}$. Each curve in Fig.(3-11) is for a given $\mathbf{k}_{||}$, in other words for a given angle measured from the direction of incidence of the photon. The intensity is plotted as a function of the energy of the outgoing electron. The zero corresponds to an electron extracted from the Fermi level. Electrons with a smaller kinetic energy come from states with larger binding energy. In other words, each of the curves above is basically

a plot of the hole-like part of $A\left(\mathbf{k}_{||},\omega\right)$. From band structure calculations, one knows that the angle $\theta = 14.75^0$ corresponds to the Fermi level (marked k_F on the plot) of a $Ti-3d$ derived band. It is for this scattering angle that the agreement between experiment and Fermi liquid theory is best (see Sec.(3.5.6) below). The plots for angles $\theta < 14.75^0$ corresponds to wave vectors above the Fermi level. There, the intensity is *much* smaller than for the other peaks. For $\theta = 13^0$, the experimental results are scaled up by a factor 16. The intensity observed for wave-vectors above the Fermi wave vector comes from the overlap of particle-like excitations with eigenstates below the Fermi surface, a phenomenon we alluded to in the previous section.

The energy resolution is $35meV$. Nevertheless, it is clear that the line shapes are larger than the energy resolution: Clearly the spectral weight is not a delta function and the electrons in the system are not free particles. Nevertheless, there is a definite maximum in the spectra whose position changes with $\mathbf{k}_{||}$. It is tempting to associate the width of the line to a lifetime. In other words, a natural explanation of these spectra is that the electrons inside the system are "quasiparticles" whose energy disperses with wave vector and that have a lifetime. We try to make these concepts more precise below.

3.5.5   Quasiparticles[17]

For a general interacting system, the one-particle Green's function takes the form,

$$G^R\left(\mathbf{k},\omega\right) = \frac{1}{\omega + i\eta - \zeta_\mathbf{k} - \sum^R\left(\mathbf{k},\omega\right)} \tag{3.196}$$

The corresponding spectral weight is,

$$A\left(\mathbf{k},\omega\right) = -2\operatorname{Im}G^R\left(\mathbf{k},\omega\right) \tag{3.197}$$

$$= \frac{-2\operatorname{Im}\sum^R\left(\mathbf{k},\omega\right)}{\left(\omega - \zeta_\mathbf{k} - \operatorname{Re}\sum^R\left(\mathbf{k},\omega\right)\right)^2 + \left(\operatorname{Im}\sum^R\left(\mathbf{k},\omega\right)\right)^2} \tag{3.198}$$

If the imaginary part of the self-energy, the scattering rate, is not too large and varies smoothly with frequency, the spectral weight will have a maximum whenever

$$\boxed{\omega - \zeta_\mathbf{k} - \operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right) = 0} \tag{3.199}$$

Let $E_\mathbf{k} - \mu$ be the value of ω for which this equation is satisfied. $E_\mathbf{k}$ is the so-called *quasiparticle energy*. This energy is clearly in general different from the results of band structure calculations that are usually obtained by neglecting the frequency dependence of the self-energy. Expanding $\omega - \zeta_\mathbf{k} - \operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right)$ around $\omega - E_\mathbf{k} + \mu$ where $A\left(\mathbf{k},\omega\right)$ is a maximum, we find

$$\omega - \zeta_\mathbf{k} - \operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right) \approx \left(1 - \left.\frac{\partial\operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right)}{\partial\omega}\right|_{E_\mathbf{k} - \mu}\right)\left(\omega - E_\mathbf{k} + \mu\right) + \ldots \tag{3.200}$$

If we define the "quasiparticle weight" or square of the wave function renormalization by

$$\boxed{Z_\mathbf{k} = \frac{1}{1 - \frac{\partial}{\partial\omega}\left.\operatorname{Re}\Sigma^R\left(\mathbf{k},\omega\right)\right|_{\omega = E_\mathbf{k} - \mu}}} \tag{3.201}$$

then in the vicinity of the maximum, the spectral weight takes the following simple form in the vicinity of the Fermi level, where the peak is sharpest

$$A\left(\mathbf{k},\omega\right) \approx 2\pi Z_{\mathbf{k}}\frac{1}{\pi}\frac{-Z_{\mathbf{k}}\operatorname{Im}\sum^{R}\left(\mathbf{k},\omega\right)}{\left(\omega - E_{\mathbf{k}}+\mu\right)^{2}+\left(Z_{\mathbf{k}}\operatorname{Im}\sum^{R}\left(\mathbf{k},\omega\right)\right)^{2}} + inc \quad (3.202)$$

$$= 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}\left(\omega\right)}{\left(\omega - E_{\mathbf{k}}+\mu\right)^{2}+\left(\Gamma_{\mathbf{k}}\left(\omega\right)\right)^{2}}\right] + inc \quad (3.203)$$

The last equation needs some explanation. First, it is clear that we have defined the scattering rate

$$\boxed{\Gamma_{\mathbf{k}}\left(\omega\right) = -Z_{\mathbf{k}}\operatorname{Im}\Sigma^{R}\left(\mathbf{k},\omega\right)} \quad (3.204)$$

Second, the quantity in square brackets looks, as a function of frequency, like a Lorentzian. At least if we can neglect the frequency dependence of the scattering rate. The integral over frequency of the square bracket is unity. Since $A\left(\mathbf{k},\omega\right)/2\pi$ is normalized to unity, this means both that

$$Z_{\mathbf{k}} \leq 1 \quad (3.205)$$

and that there are additional contributions to the spectral weight that we have denoted *inc* in accord with the usual terminology of "incoherent background". The equality in the last equation holds only if the real part of the self-energy is frequency independent.

It is also natural to ask how the quasiparticle disperses, in other words, what is its effective Fermi velocity compared with that of the bare particle. Let us define the bare velocity by

$$v_{\mathbf{k}} = \nabla_{\mathbf{k}}\zeta_{\mathbf{k}} \quad (3.206)$$

and the renormalized velocity by

$$v_{\mathbf{k}}^{*} = \nabla_{\mathbf{k}}E_{\mathbf{k}} \quad (3.207)$$

Then the relation between both quantities is easily obtained by taking the gradient of the quasiparticle equation Eq.(3.199)

$$\nabla_{\mathbf{k}}\left[E_{\mathbf{k}} - \mu - \zeta_{\mathbf{k}} - \operatorname{Re}\Sigma^{R}\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right) = 0\right] \quad (3.208)$$

$$v_{\mathbf{k}}^{*} - v_{\mathbf{k}} - \nabla_{\mathbf{k}}\operatorname{Re}\Sigma^{R}\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right) - \left.\frac{\partial\operatorname{Re}\Sigma^{R}\left(\mathbf{k},\omega\right)}{\partial\omega}\right|_{E_{\mathbf{k}}-\mu}v_{\mathbf{k}}^{*} = 0 \quad (3.209)$$

where $\nabla_{\mathbf{k}}$ in the last equation acts only on the first argument of $\operatorname{Re}\Sigma^{R}\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right)$. The last equation is easily solved if we can write that $\mathbf{k}$ dependence of Σ^{R} as a function of $\zeta_{\mathbf{k}}$ instead, something that is always possible for spherical Fermi surfaces. In such a case, we have

$$\boxed{v_{\mathbf{k}}^{*} = v_{\mathbf{k}}\frac{1+\frac{\partial}{\partial\zeta_{\mathbf{k}}}\operatorname{Re}\Sigma^{R}\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right)}{1-\left.\frac{\partial}{\partial\omega}\operatorname{Re}\Sigma^{R}\left(\mathbf{k},\omega\right)\right|_{\omega=E_{\mathbf{k}}-\mu}}} \quad (3.210)$$

In cases where the band structure has correctly treated the $\mathbf{k}$ dependence of the self-energy, or when the latter is negligible, then the renormalized Fermi velocity differs from the bare one only through the famous quasiparticle renormalization factor. In other words, $v_{\mathbf{k}}^{*} = Z_{\mathbf{k}}v_{\mathbf{k}}$. The equation for the renormalized velocity is also often written in terms of a mass renormalization instead. Indeed, we will discuss later the fact that the Fermi wave vector k_{F} is unmodified by interactions for spherical Fermi surfaces (Luttinger's theorem). Defining then $m^{*}v_{k_{F}}^{*} = k_{F} = mv_{k_{F}}$ means that our equation for the renormalized velocity gives us

$$\boxed{\frac{m}{m^{*}} = \lim_{\mathbf{k}\to\mathbf{k}_{F}}\frac{1+\frac{\partial}{\partial\zeta_{\mathbf{k}}}\operatorname{Re}\Sigma^{R}\left(\mathbf{k}, E_{\mathbf{k}}-\mu\right)}{1-\left.\frac{\partial}{\partial\omega}\operatorname{Re}\Sigma^{R}\left(\mathbf{k},\omega\right)\right|_{\omega=E_{\mathbf{k}}-\mu}}} \quad (3.211)$$

3.5.6 Fermi liquid interpretation of ARPES

Let us see how to interpret the experiments of the previous subsection in light of the quasiparticle model just described. First of all, the wave vectors studied are all close to the Fermi surface as measured on the scale of k_F. Hence, every quantity appearing in the quasiparticle spectral weight Eq.(3.203) is evaluated for $k = k_F$ so that only the frequency dependence of the remaining quantities is important. The experiments were carried out at $T = 20K$ where the resistivity has a T^2 temperature dependence. This is the regime dominated by electron-electron interactions, where so-called Fermi liquid theory applies. What is Fermi liquid theory? It would require more than the few lines that we have to explain it, but roughly speaking, for our purposes, let us say that it uses the fact that phase space for electron-electron scattering vanishes at zero temperature and at the Fermi surface, to argue that the quasiparticle model applies to interacting electrons. Originally the model was developed by Landau for liquid ^3He which has fermionic properties, hence the name Fermi Liquid theory. It is a very deep theory that in a sense justifies all the successes of the almost-free electron picture of electrons in solids. We cannot do it justice here. A simple way to make its main ingredients plausible, [18] is to assume that near the Fermi surface, at frequencies much less than temperature, the self-energy is *i)* analytic and *ii)* has an imaginary part that vanishes at zero frequency. The latter result follows from general considerations on the Pauli principle and available phase space that we do not discuss here.

Let us define real and imaginary parts of the retarded self-energy by

$$\Sigma^R = \Sigma' + i\Sigma'' \tag{3.212}$$

Our two hypothesis imply that Σ'' has the Taylor expansion

$$\Sigma'' (\mathbf{k}_F; \omega) = \alpha\omega - \gamma\omega^2 + \dots \tag{3.213}$$

The imaginary part of the retarded self-energy must be negative to insure that the retarded Green's function has poles in the lower half-plane, as is clear from the general relation between Green function and self-energy Eq.(3.196). This means that we must have $\alpha = 0$ and $\gamma > 0$. Fermi liquid theory keeps only the leading term

$$\Sigma'' = -\gamma\omega^2$$

We will verify for simple models that this quadratic frequency dependence is essentially correct in $d \geq 3$. The real part is then obtained from the Kramers-Kronig relation Eq.(**??**), (Sec.3.6.2) or from the spectral representation,

$$
\lim_{\omega \to 0} [\Sigma' (\mathbf{k}_F; \omega) - \Sigma' (\mathbf{k}_F; \infty)] = \lim_{\omega \to 0} \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma'' (\mathbf{k}_F; \omega')}{\omega' - \omega} \tag{3.214}
$$

$$
= \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma'' (\mathbf{k}_F; \omega')}{\omega'} + \omega \left[\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma'' (\mathbf{k}_F; \omega')}{(\omega')^2} \right] \tag{3.215}
$$

The first term is the value of the real-part of the self-energy at zero-frequency. This constant contributes directly to the numerical value of the chemical potential (the Hartree-Fock shift $\Sigma' (\mathbf{k}_F; \infty)$ does not suffice to evaluate the chemical potential). The second term in the last equation tells us that

$$
\frac{\partial}{\partial\omega}\Sigma' (\mathbf{k}_F, \omega)\bigg|_{\omega=0} = \left[\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\Sigma'' (\mathbf{k}_F; \omega')}{(\omega')^2} \right] \tag{3.216}
$$

Since $\Sigma'' = -\gamma\omega^2$ the integral exists and is negative (if we assume a frequency cutoff as discussed below), hence

$$\left.\frac{\partial}{\partial\omega}\Sigma'\left(\mathbf{k},\omega\right)\right|_{\omega=0} < 0 \qquad (3.217)$$

This in turn means that the corresponding value of Z_{k_F} is less than unity, as we had concluded in Eqs.(3.201) and (3.205) above. In summary, the analyticity hypothesis along with the vanishing of $\Sigma''(0)$ implies the existence of quasiparticles.

Remark 44 *Warning: there are subtleties. The above results assume that there is a cutoff to $\Sigma''\left(\mathbf{k}_F;\omega'\right)$. The argument just mentioned in Eq.(3.216) fails when the integral diverges. Then, the low frequency expansion for the self-energy in Eq.(3.215) cannot be done. Expanding under the integral sign is no longer valid. One must do the principal part integral first. In fact, even for a Fermi liquid at finite temperature, $\Sigma''\left(\mathbf{k}_F;\omega\right) \sim \omega^2 + \left(\pi T\right)^2$ so that the $\left(\pi T\right)^2$ appears to lead to a divergent integral in Eq.(3.216). Returning to the original Kramers-Krönig expression fo Σ' however, the principal part integral shows that the constant term $\left(\pi T\right)^2$ for $\Sigma''\left(\mathbf{k}_F;\omega\right)$ does not contribute at all to Σ' if the cutoff in Σ'' is symmetric at positive and negative frequencies. In practice one can encounter situations where $\partial\Sigma/\partial\omega > 0$. In that case, we do not have a Fermi liquid since $Z > 1$ is inconsistent with the normalization of the spectral weight. One can work out an explicit example in the renormalized classical regime of spin fluctuations in two dimensions. (Appendix D of [28]).*

The solid lines in Fig.(3-11) are two-parameter fits that also take into account the wave vector and energy resolution of the experiment [19]. One parameter is $E_k - \mu$ while the other one is γ', a quantity defined by substituting the Fermi liquid approximation in the equation for damping Eq.(3.204)

$$\Gamma_{k_F}\left(\omega\right) = Z_{k_F}\gamma\omega^2 = \gamma'\omega^2. \qquad (3.218)$$

Contrary to E_k, the damping parameter γ' is the same for all curves. The solid-line fits are obtained with $\gamma' = 40eV^{-1}$ (β' on the figure). The fits become increasingly worse as one moves away from the Fermi surface, as expected. It is important to notice, however, that even the small left-over weight for wave-vectors above the Fermi surface $\left(\theta < 14.75^0\right)$ can be fitted with the same value of γ. This weight is the tail of a quasiparticle that could be observed at positive frequencies in inverse photoemission experiments (so-called BIS). The authors compared the results of their fits to the theoretical estimate,[20] $\gamma = 0.067\omega_p/\varepsilon_F^2$. Using $\omega_p = 18.2eV$, $\varepsilon_F = 0.3eV$ and the extrapolated value of Z_{k_F} obtained by putting[2] $r_s = 10$ in electron gas results,[21] they find $\gamma' < 5\left(eV\right)^{-1}$ while their experimental results are consistent with $\gamma' = 40 \pm 5\left(eV\right)^{-1}$. The theoretical estimate is almost one order of magnitude smaller than the experimental result. This is not so bad given the crudeness of the theoretical model (electron gas with no lattice effect). In particular, this system is a semimetal so that there are other decay channels than just the one estimated from a single circular Fermi surface. Furthermore, electron gas calculations are formally correct only for small r_s while there we have $r_s = 10$.

More recent experiments have been performed by Grioni's group [27]. Results are shown in Fig. (3-12). In this work, authors allow for a constant damping $\Gamma_0 = 17\ meV$ coming from the temperature and from disorder and then they fit the rest with a Fermi velocity $\hbar v_F = 0.73 \pm 0.1eV\ \mathring{A}$ close to band structure calculations, $\hbar v_F = 0.68\ eV\ \mathring{A}$ and γ' that varies between $0.5\ eV^{-1}$ $\left(16^0\right)$ and $0.9\ eV^{-1}$ $\left(14.5^0\right)$. The Fermi liquid fit is just as good, but the interpretation of the origin of the broadening terms is different. This shows that there is much uncertainty still in the interpretation of ARPES data, even for Fermi liquids.

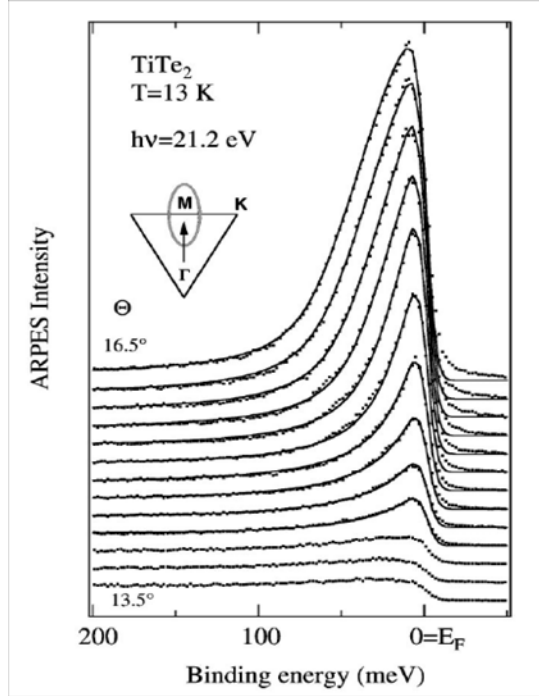[2] r_s is the average electron spacing expressed in terms of the Bohr radius.

Figure 3-12   Figure 1 from Ref.[27] for the ARPES spectrum of 1T-TiTe$_2$ measured near the Fermi surface crossing along the high-symmetry ΓM direction ($\theta = 0$ is normal emission). The lines are results of Fermi liquid fits and the inset shows a portion of the Brillouin zone with the relevant ellipsoidal electron pocket.

Theoretical estimates for high-temperature superconductors are two orders of magnitude smaller than the observed result [19].

Remark 45 *Asymmetry of the lineshape: The line shapes are asymmetrical, with a tail at energies far from the Fermi surface (large binding energies). This is consistent with the fact that the "inverse lifetime" $\Gamma_{k_F}(\omega) = Z_{k_F}\gamma\omega^2$ is not a constant, but is instead larger at larger binding energies.*

Remark 46 *Failure of Fermi liquid at high-frequency: Clearly the Fermi liquid expression for the self-energy fails at large frequencies since we know from its spectral representation that the real-part of the self-energy goes to a frequency-independent constant at large frequency, the first correction being proportional to $1/ik_n$ as discussed below in subsection (3.6.1). Conversely, there is always a cutoff in the imaginary part of the self-energy. This is not apparent in the Fermi liquid form above but we had to assume its existence for convergence. The cutoff on the imaginary part is analogous to the cutoff in χ''. Absorption cannot occur at arbitrary high frequency.*

Remark 47 *Destruction of quasiparticles by critical fluctuations in two dimensions: Note that it is only if Σ'' vanishes fast enough with frequency that it is correct to expand the Kramers-Kronig expression in powers of the frequency to obtain Eq.(3.216). When $\Sigma''(\omega)$ vanishes slower than ω^2, then Eq.(3.216) for the slope of the real part is not valid. The integral does not converge uniformly and it is not possible to interchange the order of differentiation and integration. In such a case it is possible to have the opposite inequality for the slope of the real part $\frac{\partial}{\partial \omega}\Sigma'(\mathbf{k},\omega)\big|_{\omega=0} > 0$. This does not lead to any contradiction, such as $Z_{k_F} > 1$,*

because there is no quasiparticle solution at $\omega = 0$ in this case. This situation occurs for example in two dimensions when classical thermal fluctuations create a pseudogap in the normal state before a zero-temperature phase transition is reached [22].

3.5.7 Momentum distribution in an interacting system

In an interacting system, momentum is not a good quantum number so $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ is *not* equal to the Fermi distribution. On the other hand, $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ can be computed from the spectral weight. Indeed,

$$\begin{aligned} \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle &= \lim_{\tau \to 0^-} \left[-\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger} \right\rangle \right] \\ &= \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) \end{aligned} \quad (3.219)$$

To compute the latter quantity from the spectral weight, it suffices to use the spectral representation Eq.(3.122)

$$\begin{aligned} \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) &= T \lim_{\tau \to 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \\ &= T \lim_{\tau \to 0^-} \sum_{n=-\infty}^{\infty} e^{-ik_n \tau} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}, \omega')}{ik_n - \omega'} \end{aligned} \quad (3.220)$$

Using the result Eq.(3.163) found above for the sum over Matsubara frequencies, we are left with

$$\boxed{\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \lim_{\tau \to 0^-} \mathcal{G}(\mathbf{k}, \tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega') A(\mathbf{k}, \omega')} \quad (3.221)$$

with $f(\omega')$ the Fermi-Dirac distribution.

This means that the momentum distribution is a Fermi-Dirac distribution only if the spectral weight is a delta function. This occurs for free particles or, more generally if the real-part of the self-energy is frequency independent since, in this case, the Kramers-Kronig relations imply that the imaginary part of the self-energy vanishes so that Eq.(3.198) for the spectral weight gives us a delta function.

Remark 48 *Jump of the momentum distribution at the Fermi level: Even if $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ is no-longer a Fermi-Dirac distribution in an interacting system, nevertheless at zero-temperature in a system subject only to electron-electron interaction, there is a jump in $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle$ at the Fermi level. The existence of this jump can be seen as follows. At zero temperature, our last result gives us*

$$\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \int_{-\infty}^{0} \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega') \quad (3.222)$$

Let us take the quasiparticle form Eq.(3.203) of the spectral weight with the Fermi liquid expression Eq.(3.218) for the scattering rate. The incoherent background varies smoothly with $\mathbf{k}$ and hence cannot lead to any jump in occupation number. The quasiparticle piece on the other hand behaves when $k \to k_F$, or in other words when $E_{\mathbf{k}} - \mu \to 0$, as $Z_{k_F} \delta(\omega)$. At least crudely speaking. When $E_{\mathbf{k}} - \mu \to 0^-$, this

delta function is inside the integration domain hence it contributes to the integral, while when $E_{\mathbf{k}} - \mu \to 0^+$ the delta function is outside and does not contribute to the integral. This means that there is a big difference between these two nearby wave vectors, namely

$$\lim_{\mathbf{k}\to\mathbf{k}_f^-} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle - \lim_{\mathbf{k}\to\mathbf{k}_f^+} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle = Z_{k_F} \tag{3.223}$$

In the above argument, we have done as if $\Gamma_{\mathbf{k}}(\omega)$ was frequency independent and infinitesimally small in Eq.(3.203). This is not the case so our argument is rather crude. Nevertheless, if one uses the actual frequency-dependent forms and does the frequency integral explicitly, one can check that the above conclusion about the jump is true (although less trivial).

Remark 49 *Fermi surface and interactions: The conclusion of the previous remark is that even in an interacting system, there is a sharp Fermi surface as in the free electron model. For simplicity we have discussed the spinless case. A qualitative sketch of the zero-temperature momentum distribution in an interacting system appears in Fig.(3-13). Since momentum of a single particle is not a good quantum number anymore, some states above the Fermi momentum are now occupied while others below are empty. Nevertheless, the Fermi surface is unaffected.*
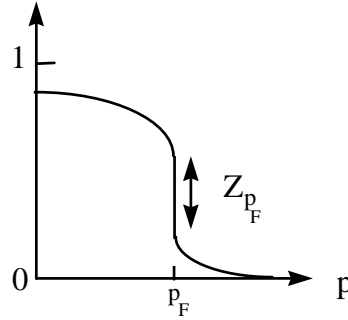
Figure 3-13   Qualitative sketch of the zero-temperature momentum distribution in an interacting system.

Remark 50 *Luttinger's theorem: More generally, in a Fermi liquid the volume of reciprocal space contained within the Fermi surface defined by the jump, is independent of interactions. This is Luttinger's theorem. In the case where the Fermi surface is spherical, this means that k_F is unaffected.*

3.6   A few more formal matters : asymptotic behavior and causality

In designing approximations, we have to try to preserve as many as possible of the exact properties. Sum rules are such properties. They determine the structure of the high-frequency expansion and hence one can also check whether a given approximation preserves the sum rules by looking at its high-frequency expansion.

This is the first topic we will discuss. The second topic concerns restrictions imposed by causality. This has become a very important topic in the context of Dynamical Mean-field theory or other approaches that describe the physics that occurs at strong coupling, such as the Mott transition. We will come back on this in later chapters.

3.6.1 Asymptotic behavior of $\mathcal{G}(\mathbf{k};ik_n)$ and $\Sigma(\mathbf{k};ik_n)$

As usual, the high-frequency asymptotic properties of the Green's function are determined by sum rules. From the spectral representation(3.122), we obtain, for the general interacting case

$$\lim_{ik_n \to \infty} \mathcal{G}(\mathbf{k};ik_n) = \lim_{ik_n \to \infty} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k};\omega')}{ik_n - \omega'} \tag{3.224}$$

$$= \lim_{ik_n \to \infty} \frac{1}{ik_n} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k};\omega') = \lim_{ik_n \to \infty} \frac{1}{ik_n} \left\langle \{c_{\mathbf{k}}, c_{\mathbf{k}}^+\} \right\rangle = \lim_{ik_n \to \infty} \frac{1}{ik_n} \tag{3.225}$$

Defining the self-energy as usual

$$\mathcal{G}(\mathbf{k};ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k},ik_n)} \tag{3.226}$$

the correct asymptotic behavior for the Green's function implies that the self-energy at high frequency cannot diverge: It must go to a constant independent of frequency

$$\lim_{ik_n \to \infty} \Sigma(\mathbf{k},ik_n) = cst. \tag{3.227}$$

We will see later that the value of this constant is in fact given correctly by the Hartree-Fock approximation.

The converse of the above result [18] for the Green's function, is that if

$$\lim_{ik_n \to \infty} \mathcal{G}(\mathbf{k};ik_n) = \lim_{ik_n \to \infty} \frac{1}{ik_n}$$

then that is all that is needed to obtain an approximation for the Green's function which obeys the anticommutation relation:

$$\mathcal{G}(\mathbf{k};0^-) - \mathcal{G}(\mathbf{k};0^+) = \langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \rangle + \langle c_{\mathbf{k}} c_{\mathbf{k}}^+ \rangle = 1 \tag{3.228}$$

Proof :It suffices to notice that

$$\mathcal{G}(\mathbf{k};0^-) - \mathcal{G}(\mathbf{k};0^+) = \frac{1}{\beta} \sum_n \left[e^{-ik_n 0^-} - e^{-ik_n 0^+} \right] \mathcal{G}(\mathbf{k};ik_n) \tag{3.229}$$

We can add and subtract the asymptotic behavior to obtain,

$$\frac{1}{\beta} \sum_n \left[\left(e^{-ik_n 0^-} - e^{-ik_n 0^+} \right) \left(\mathcal{G}(\mathbf{k};ik_n) - \frac{1}{ik_n} \right) \right] + \frac{1}{\beta} \sum_n \left(e^{-ik_n 0^-} - e^{-ik_n} \right) \frac{1}{ik_n}$$

$$\tag{3.230}$$

In the first sum, $\mathcal{G}(\mathbf{k};ik_n) - \frac{1}{ik_n}$ decays faster than $\frac{1}{ik_n}$ so that the convergence factors are not needed for the sum to converge. This means that this first sum vanishes. The last sum gives unity, as we easily see from the previous section. This proves our assertion.

Remark 51 *High-frequency expansion for the Green's function and sum-rules: The coefficients of the high-frequency expansion of $\mathcal{G}(\mathbf{k}; ik_n)$ in powers of $1/ik_n$ are obtained from sum rules on the spectral weight, in complete analogy with what we have found in previous chapters. The fact that $A(\mathbf{k}, \omega)$ falls fast enough to allow us to expand under the integral sign follows from the fact that all frequency moments of $A(\mathbf{k}, \omega)$, namely $\int d\omega \omega^n A(\mathbf{k}, \omega)$, exist and are given by equal-time commutators. Explicit expressions for $A(\mathbf{k}, \omega)$ in terms of matrix elements, as given in Subsection(3.5.3) above, show physically why $A(\mathbf{k}, \omega)$ falls so fast at large frequencies. As an example, to show that the coefficient of the $1/ik_n$ term in the high frequency expansion is equal to $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega')$ it is sufficient that $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} |\omega' A(\mathbf{k}; \omega')|$ exists.[16] This can be seen as follows,*

$$ik_n \mathcal{G}(\mathbf{k}; ik_n) - \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \quad = \quad \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \left(\frac{ik_n}{ik_n - \omega'} - 1 \right) \tag{3.231}$$

$$= \quad \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \frac{\omega'}{ik_n - \omega'} \tag{3.232}$$

$$\leq \quad \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left| A(\mathbf{k}; \omega') \frac{\omega'}{ik_n - \omega'} \right| \tag{3.233}$$

$$\leq \quad \left| \frac{1}{ik_n} \right| \left| \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} |A(\mathbf{k}; \omega') \omega'| \right. \tag{3.234}$$

If the integral exists then, it is a rigorous result that

$$\lim_{ik_n \to \infty} ik_n \mathcal{G}(\mathbf{k}; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \tag{3.235}$$

This is an important result. It suggests that approximate theories that give 1 as the coefficient of $(ik_n)^{-1}$ in the high frequency expansion have a normalized spectral weight. However[16] the above proof assumes that there is indeed a spectral representation for $\mathcal{G}(\mathbf{k}; ik_n)$. A Green's function for a theory that is not causal fails to have a spectral representation. If a spectral representation is possible, the analytically continued approximate $G^R(\mathbf{k}, \omega)$ is necessarily causal. Approximate theories may not be causal. This failure of causality may reflect a phase transition, as we will see later, or may simply be a sign that the approximation is bad. As an example, suppose that we obtain $\mathcal{G}(\mathbf{k}; ik_n) = (ik_n - ia)^{-1}$. This has the correct high-frequency behavior but its analytical continuation does not satisfy causality. It has no spectral representation. On the other hand, $\mathcal{G}(\mathbf{k}; ik_n) = (ik_n + (k_n/|k_n|)ia)^{-1}$ has a Lorentzian as a spectral weight and is causal. It may also occur that the approximate theory may have $\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') = 1$ but $A(\mathbf{k}; \omega') < 0$ for some range of ω'. This unphysical result may again signal that the approximate theory fails because of a phase transition or because it is a bad approximation.

3.6.2 Implications of causality for G^R and Σ^R

Consider the retarded Green function as a matrix in $\mathbf{r}, \mathbf{r}'$. We will show that the real and imaginary parts of G^R and of Σ^R are each Hermitian matrices. in addition, $\mathrm{Im}\, G^R$ and $\mathrm{Im}\, \Sigma^R$ are both negative definite (except in the special case of non-interacting particles where $\mathrm{Im}\, \Sigma^R = 0$).

In analogy with the Matsubara Green function Eq.(3.180) G^R has the Lehman representation

$$G^R(\mathbf{r}, \mathbf{r}'; \omega) = e^{\beta\Omega} \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n} \right) \frac{\langle n| \psi_S(\mathbf{r}) |m \rangle \langle m| \psi_S^\dagger(\mathbf{r}') |n \rangle}{\omega + i\eta - (E_m - E_n - \mu)}. \tag{3.236}$$

Taking the complex conjugate of the transpose, we obtain

$$
\begin{aligned}
\operatorname{Re} G^R \left(\mathbf{r}', \mathbf{r}; \omega\right)^* &= e^{\beta\Omega} \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \frac{\langle n| \psi_S \left(\mathbf{r}'\right) |m\rangle^* \langle m| \psi_S \left(\mathbf{r}\right) |n\rangle^*}{\omega - \left(E_m - E_n - \mu\right)} \\
&= \operatorname{Re} G^R \left(\mathbf{r}, \mathbf{r}'; \omega\right) \qquad\qquad (3.237) \\
\operatorname{Im} G^R \left(\mathbf{r}', \mathbf{r}; \omega\right)^* &= -\pi \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \langle n| \psi_S \left(\mathbf{r}'\right) |m\rangle^* \langle m| \psi_S \left(\mathbf{r}\right) |n\rangle^* \\
&\quad \times \delta \left(\omega - \left(E_m - E_n - \mu\right)\right) \qquad\qquad (3.238) \\
&= \operatorname{Im} G^R \left(\mathbf{r}, \mathbf{r}'; \omega\right) \qquad\qquad (3.239)
\end{aligned}
$$

which means that the real and imaginary parts are both Hermitian matrices. In a basis where the matrix $\operatorname{Im} G^R \left(\mathbf{r}, \mathbf{r}'; \omega\right)$ is diagonal, say for quantum number α, then

$$
\begin{aligned}
\operatorname{Im} G^R \left(\boldsymbol{\alpha}; \omega\right) &= -\pi \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) \langle n| c_{\boldsymbol{\alpha}} |m\rangle \langle m| c_{\boldsymbol{\alpha}}^\dagger |n\rangle \delta \left(\omega - \left(E_m - E_n - \mu\right)\right) \\
&= -\pi \sum_{mn} \left(e^{-\beta K_m} + e^{-\beta K_n}\right) |\langle n| c_{\boldsymbol{\alpha}} |m\rangle|^2 \delta \left(\omega - \left(E_m - E_n - \mu\right)\right) \quad (3.240)
\end{aligned}
$$

which proves that the matrix for the imaginary part is negative definite in addition to being Hermitian. The negative sign comes from the $+i\eta$ in the original formula and is clearly a consequence of causality.

Following Potthoff [26] we show that the retarded self-energy as a matrix has the same properties as G^R. First, we need to prove that

$$
\frac{1}{A \pm iB} = X \mp iY \qquad\qquad (3.241)
$$

with X and Y both Hermitian and Y positive definite if A and B are both Hermitian with B positive definite. This is true because

$$
\frac{1}{A \pm iB} = B^{-1/2} \frac{1}{B^{-1/2} A B^{-1/2} \pm iI} B^{-1/2}. \qquad\qquad (3.242)
$$

Since $B^{-1/2} A B^{-1/2}$ is Hermitian as well, we can diagonalize it by a unitary transformation $B^{-1/2} A B^{-1/2} = U c U^\dagger$ where c is a diagonal matrix. Thus,

$$
\frac{1}{A \pm iB} = B^{-1/2} U \frac{1}{c \pm iI} U^\dagger B^{-1/2} = B^{-1/2} U \frac{c \mp iI}{c^2 + 1} U^\dagger B^{-1/2} = X \mp iY \quad (3.243)
$$

with X and Y Hermitians since $\left(U^\dagger B^{-1/2}\right)^\dagger = B^{-1/2} U$. In addition, Y is positive definite since in the diagonal basis $Y \to \left(c^2 + 1\right)^{-1}$. Now, define $\left(G^R\right)^{-1} = \left(A - iB\right)^{-1} = X + iY$ and $\left(G_0^R\right)^{-1} = \left(A_0 - iB_0\right)^{-1} = X_0 + iY_0$ so that

$$
\left(G^R\right)^{-1} = X + iY = \left(G_0^R\right)^{-1} - \Sigma^R = X_0 + iY_0 - \operatorname{Re} \Sigma^R - i \operatorname{Im} \Sigma^R. \qquad (3.244)
$$

Then, given that X, Y and X_0, Y_0 are Hermitians, we have that $\operatorname{Re} \Sigma^R$ and $\operatorname{Im} \Sigma^R$ are Hermitians. In addition, $\operatorname{Im} \Sigma^R$ is negative definite since Y_0 is infinitesimal which implies that $Y - Y_0$ can only be positive (or vanish in the non-interacting case).

3.7   Three general theorems

Risking to wear your patience out, we still have to go through three general theorems used repeatedly in Many-Body theory. Wick's theorem forms the basis ot

the diagram technique in many-body theory. The linked-cluster theorems, or cumulant expansions, are much more general theorems that are also necessary to set up the machinery of diagrams. Finally, we state a variational principle for the free energy that allows us to give a physical meaning to Hartree-Fock theory as the best one-body Hamiltonian for any given problem. This variational principle is useful for ordinary system, but also becomes indispensable when there is a broken symmetry.

3.7.1 Wick's theorem

Wick's theorem allows us to compute arbitrary correlation functions of any Hamiltonian that is quadratic in Fermion or Boson operators. That is clearly what we need to do perturbation theory, but let us look in a bit more details at how this comes about. We have already talked about Wick's theorem in the context of Hartree-Fock theory. Here we present the more general result valid at finite temperature. We will need to compute in the interaction picture

$$\mathcal{G}(\tau) = -\frac{Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{U}(\beta,\tau)\widehat{\psi}(\tau)\widehat{U}(\tau,0)\widehat{\psi}^\dagger(0)\right)\right]}{Tr\left[e^{-\beta H_0}T_\tau\widehat{U}(\beta,0)\right]} \tag{3.245}$$

Because $\widehat{U}(\tau,0)$ always contains an even number of fermions, it can be commuted with creation-annihilation operators without paying the price of minus signs so that

$$\boxed{\mathcal{G}(\tau) = -\frac{Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{U}(\beta,0)\widehat{\psi}(\tau)\widehat{\psi}^\dagger(0)\right)\right]}{Tr\left[e^{-\beta H_0}T_\tau\widehat{U}(\beta,0)\right]}} \tag{3.246}$$

More specifically the evolution operator is,

$$\boxed{\widehat{U}(\beta,0) = T_\tau\left[\exp\left(-\int_0^\beta d\tau_1\widehat{V}(\tau_1)\right)\right]} \tag{3.247}$$

Expanding this evolution operator to first order in the numerator of the Green's function one obtains

$$-Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{\psi}(\tau)\widehat{\psi}^\dagger(0)\right)\right] + \int_0^\beta d\tau_1 Tr\left[e^{-\beta H_0}T_\tau\left(\widehat{V}(\tau_1)\widehat{\psi}(\tau)\widehat{\psi}^\dagger(0)\right)\right] \tag{3.248}$$

where in the case of a two-body interaction (Coulomb for example), $\widehat{V}(\tau_1)$ contains four field operators.

Wick's theorem allows us to evaluate expectation values such as those above. More generally, it allows us to compute expectation values of creation-annihilation operators such as,

$$\left\langle a_i(\tau_i)a_j(\tau_j)a_k^\dagger(\tau_k)a_l^\dagger(\tau_l)\right\rangle_0 \tag{3.249}$$

as long as the density matrix $e^{-\beta H_0}$ is that of a quadratic Hamiltonian.

Note that since quadratic Hamiltonians conserve the number of particles, expectation values vanish when the number of creation operators does not match the number of destruction operators.

Lemma 9 *If $H_0 = \varepsilon_1 a_1^\dagger a_1 + \varepsilon_2 a_2^\dagger a_2$ then $\left\langle a_1 a_1^\dagger a_2 a_2^\dagger\right\rangle = \left\langle a_1 a_1^\dagger\right\rangle\left\langle a_2 a_2^\dagger\right\rangle$.*

Proof: To understand what is going on, it is instructive to study first the problem where a single fermion state can be occupied. Then

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{Tr\left[e^{-\beta H_0} a_1 a_1^\dagger\right]}{Tr\left[e^{-\beta H_0}\right]} \tag{3.250}$$

$$= \frac{\langle 0| a_1 a_1^\dagger |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right) a_1 a_1^\dagger \left(a_1^\dagger |0\rangle\right)}{\langle 0| |0\rangle + e^{-\beta\epsilon_1}\left(\langle 0| a_1\right)\left(a_1^\dagger |0\rangle\right)} = \frac{1}{1 + e^{-\beta\epsilon_1}} \tag{3.251}$$

For two fermion states $1, 2$, then the complete set used to evaluate the trace is

$$|0\rangle |0\rangle, \quad a_1^\dagger |0\rangle |0\rangle, \quad |0\rangle a_2^\dagger |0\rangle, \quad a_1^\dagger |0\rangle a_2^\dagger |0\rangle \tag{3.252}$$

so that

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1 + e^{-\beta\epsilon_1}} \frac{1 + e^{-\beta\epsilon_2}}{1 + e^{-\beta\epsilon_2}} = \frac{1}{1 + e^{-\beta\epsilon_1}}. \tag{3.253}$$

The easiest way to understand the last result is to recall that $\left(1 + a_1^\dagger\right)\left(1 + a_2^\dagger\right)|0\rangle$ will generate the trace so that we can factor each subspace. The last result will remain true for an arbitrary number of fermion states, in other words

$$\left\langle a_1 a_1^\dagger \right\rangle = \frac{1}{1 + e^{-\beta\epsilon_1}} \frac{\prod_{m\neq 1} 1 + e^{-\beta\epsilon_m}}{\prod_{m\neq 1} 1 + e^{-\beta\epsilon_m}} = \frac{1}{1 + e^{-\beta\epsilon_1}}. \tag{3.254}$$

Furthermore,

$$\left\langle a_1 a_1^\dagger a_2 a_2^\dagger \right\rangle = \frac{1}{1 + e^{-\beta\epsilon_1}} \frac{1}{1 + e^{-\beta\epsilon_2}} \frac{\prod_{m\neq 1,2} 1 + e^{-\beta\epsilon_m}}{\prod_{m\neq 1,2} 1 + e^{-\beta\epsilon_m}} \tag{3.255}$$

$$= \frac{1}{1 + e^{-\beta\epsilon_1}} \frac{1}{1 + e^{-\beta\epsilon_2}} \tag{3.256}$$

$$= \left\langle a_1 a_1^\dagger \right\rangle \left\langle a_2 a_2^\dagger \right\rangle \tag{3.257}$$

Theorem 10 *Any expectation value such as* $\left\langle a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0$ *calculated with a density matrix* $e^{-\beta K_0}$ *that is quadratic in field operators can be computed as the sum of all possible products of the type* $\left\langle a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \left\langle a_i\left(\tau_i\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0$ *that can be formed by pairing creation an annihilation operators. For a given term on the right-hand side, there is a minus sign if the order of the operators is an odd permutation of the order of operators on the left-hand side.*

Proof: It is somewhat pretentious to call a proof the plausibility argument that we give below, but let us go ahead anyway. The trick to prove the theorem([23]) is to transform the operators to the basis where H_0 is diagonal, to evaluate the expectation values, then to transform back to the original basis. Let Greek letters stand for the basis where H_0 is diagonal. Using the formula for basis changes, we have, (with an implicit sum over Greek indices)

$$\left\langle a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 = \tag{3.258}$$

$$\langle i| \alpha\rangle \langle j| \beta\rangle \left\langle a_\alpha\left(\tau_i\right) a_\beta\left(\tau_j\right) a_\gamma^\dagger\left(\tau_k\right) a_\delta^\dagger\left(\tau_l\right)\right\rangle_0 \langle \gamma| k\rangle \langle \delta| l\rangle \tag{3.259}$$

We already know from Eq.(3.141) that

$$a_\alpha\left(\tau_i\right) = e^{-\zeta_\alpha \tau_i} a_\alpha \quad ; \quad a_\alpha^\dagger\left(\tau_i\right) = a_\alpha^\dagger e^{\zeta_\alpha \tau_i} \tag{3.260}$$

so that

$$\left\langle a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 \qquad (3.261)$$

$$= \left\langle i\middle| \alpha\right\rangle e^{-\zeta_\alpha \tau_i} \left\langle j\middle| \beta\right\rangle e^{-\zeta_\beta \tau_j} \left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 e^{\zeta_\gamma \tau_k} \left\langle\gamma\middle| k\right\rangle e^{\zeta_\delta \tau_l} \left\langle\delta\middle| l\right\rangle \quad (3.262)$$

What we need to evaluate then are expectation values of the type

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0. \qquad (3.263)$$

Evaluating the trace in the diagonal basis, we see that we will obtain a non-zero value only if indices of creation and annihilation operators match two by two or are all equal. Suppose $\beta = \gamma$, $\alpha = \delta$ and $\alpha \neq \beta$. Then, as in the lemma

$$\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0 = \left\langle a_\alpha a_\alpha^\dagger\right\rangle_0 \left\langle a_\beta a_\beta^\dagger\right\rangle_0 \qquad (3.264)$$

If instead, $\beta = \delta$, $\alpha = \gamma$ and $\alpha \neq \beta$, then

$$\left\langle a_\alpha a_\beta a_\alpha^\dagger a_\beta^\dagger\right\rangle_0 = -\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0 = -\left\langle a_\alpha a_\alpha^\dagger\right\rangle_0 \left\langle a_\beta a_\beta^\dagger\right\rangle_0. \qquad (3.265)$$

The last case to consider is $\alpha = \beta$, $\beta = \delta$, $\alpha = \gamma$

$$\left\langle a_\alpha a_\alpha a_\alpha^\dagger a_\alpha^\dagger\right\rangle_0 = 0. \qquad (3.266)$$

All these results, Eqs.(3.264)(3.265) and the last equation can be combined into one formula

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 = \left\langle a_\alpha a_\alpha^\dagger\right\rangle_0 \left\langle a_\beta a_\beta^\dagger\right\rangle_0 \left(\delta_{\alpha,\delta}\delta_{\beta,\gamma} - \delta_{\alpha,\gamma}\delta_{\beta,\delta}\right) \quad (3.267)$$

$$= \left\langle a_\alpha a_\delta^\dagger\right\rangle_0 \left\langle a_\beta a_\gamma^\dagger\right\rangle_0 - \left\langle a_\alpha a_\gamma^\dagger\right\rangle_0 \left\langle a_\beta a_\delta^\dagger\right\rangle_0 \qquad (3.268)$$

which is easiest to remember as follows,

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle = \left\langle \overset{\downarrow}{a_\alpha} a_\beta a_\gamma^\dagger \overset{\downarrow}{a_\delta^\dagger}\right\rangle + \left\langle \overset{\downarrow}{a_\alpha} a_\beta \overset{\downarrow}{a_\gamma^\dagger} a_\delta^\dagger\right\rangle \qquad (3.269)$$

in other words, all possible pairs of creation and annihilation operators must be paired ("contracted") in all possible ways. There is a minus sign if an odd number of operator exchanges (transpositions) is necessary to bring the contracted operators next to each other on the right-hand side (In practice, just count one minus sign every time two operators are permuted). Substituting Eq.(3.268) back into the expression for the original average expressed in the diagonal basis Eq.(3.262) we have

$$\left\langle a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 \qquad (3.270)$$

$$= \left\langle a_i\left(\tau_i\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 \left\langle a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 - \left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \left\langle a_j\left(\tau_j\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0$$

By induction (not done here) one can show that this result generalizes to the expectation value of an arbitrary number of creation-annihilation operators.

Definition 11 *Contraction: In the context of Wick's theorem, we call each factor* $\left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0$ *on the right-hand side, a "contraction".*

Since Wick's theorem is valid for an arbitrary time ordering, it is also valid for time-ordered products so that, for example

$$\boxed{\left\langle T_\tau \left[a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0 =} \tag{3.271}$$

$$\boxed{\left\langle T_\tau \left[a_i\left(\tau_i\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0 \left\langle T_\tau \left[a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 - \left\langle T_\tau \left[a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 \left\langle T_\tau \left[a_j\left(\tau_j\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0}.$$
$$\tag{3.272}$$

The only simplification that occurs with time-ordered products is the following. Note that, given the definition of time-ordered product, we have

$$\left\langle T_\tau \left[a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 = -\left\langle T_\tau \left[a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right]\right\rangle_0 \tag{3.273}$$

Indeed, the left-hand side and right-hand side of the above equation are, respectively

$$\left\langle T_\tau \left[a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 = \left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \theta\left(\tau_i - \tau_k\right) \tag{3.274}$$

$$- \left\langle a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \theta\left(\tau_k - \tau_i\right) \tag{3.275}$$

$$-\left\langle T_\tau \left[a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right]\right\rangle_0 = -\left\langle a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \theta\left(\tau_k - \tau_i\right) \tag{3.276}$$

$$+ \left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \theta\left(\tau_i - \tau_k\right) \tag{3.277}$$

In other words, operators can be permuted at will inside a time-ordered product, in particular inside a contraction, as long as we take care of the minus-signs associated with permutations. This is true for time-ordered products of an arbitrary number of operators and for an arbitrary density matrix.

On the other hand, if we apply Wick's theorem to a product that is not time ordered, then we have to remember that

$$\left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \neq -\left\langle a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \tag{3.278}$$

as we can easily verify by looking at the special case $\tau_k = \tau_i$ or by going to a diagonal basis. We can anticommute operators at will to do the "contractions" but they cannot be permuted *inside* a contraction $\left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0$.

In practice, we will apply Wick's theorem to time-ordered products. In numerical calculations it is sometimes necessary to apply it to objects that are not time-ordered.

Example 12 *To make the example of Wick's theorem Eq.(3.272) more plausible, we give a few examples, Suppose first that the time order to the left of Eq.(3.272) is such that the destruction operators are inverted. Then,*

$$\left\langle T_\tau \left[a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0 = -\left\langle a_j\left(\tau_j\right) a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 \tag{3.279}$$

which means that since i and j have exchanged roles, in doing the contractions as above there is one more permutation to do, which gets rid of the extra minus sign and reproduces the right-hand side of Eq.(3.272). More explicitly, to do the contractions as above, we have to change i for j on both the right- and the left-hand side of Eq.(3.270). Doing this and substituting above, we obtain

$$\left\langle a_j\left(\tau_j\right) a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 = \left\langle a_j\left(\tau_j\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 \left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 - \left\langle a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \left\langle a_i\left(\tau_i\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0$$
$$\tag{3.280}$$

which we substitute in the previous equation to obtain exactly what the right-hand side of Eq.(3.272) would have predicted. To take another example, suppose that the time orders are such that

$$\left\langle T_\tau \left[a_i (\tau_i) a_j (\tau_j) a_k^\dagger (\tau_k) a_l^\dagger (\tau_l) \right] \right\rangle_0 = - \left\langle a_i (\tau_i) a_k^\dagger (\tau_k) a_j (\tau_j) a_l^\dagger (\tau_l) \right\rangle_0 .$$
$$(3.281)$$

Then, to do the contractions we proceed as above, being careful not to permute creation and annihilation operators within an expectation value

$$- \left\langle a_i (\tau_i) a_k^\dagger (\tau_k) a_j (\tau_j) a_l^\dagger (\tau_l) \right\rangle_0$$
$$= - \left\langle a_i (\tau_i) a_l^\dagger (\tau_l) \right\rangle_0 \left\langle a_k^\dagger (\tau_k) a_j (\tau_j) \right\rangle_0 - \left\langle a_i (\tau_i) a_k^\dagger (\tau_k) \right\rangle_0 \left\langle a_j (\tau_j) a_l^\dagger (\tau_l) \right\rangle_0$$
$$(3.282)$$

The right-hand side of Eq.(3.272) gives us

$$\left\langle T_\tau \left[a_i (\tau_i) a_l^\dagger (\tau_l) \right] \right\rangle_0 \left\langle T_\tau \left[a_j (\tau_j) a_k^\dagger (\tau_k) \right] \right\rangle_0 - \left\langle T_\tau \left[a_i (\tau_i) a_k^\dagger (\tau_k) \right] \right\rangle_0 \left\langle T_\tau \left[a_j (\tau_j) a_l^\dagger (\tau_l) \right] \right\rangle_0$$
$$= - \left\langle a_i (\tau_i) a_l^\dagger (\tau_l) \right\rangle_0 \left\langle a_k^\dagger (\tau_k) a_j (\tau_j) \right\rangle_0 - \left\langle a_i (\tau_i) a_k^\dagger (\tau_k) \right\rangle_0 \left\langle a_j (\tau_j) a_l^\dagger (\tau_l) \right\rangle_0 \qquad (3.283)$$

with the minus sign in the first term because we had to exchange the order in one of the time-ordered products.

3.7.2 Linked cluster theorems

Suppose we want to evaluate the Green's function by expanding the time-ordered product in the evolution operator Eq.(3.247). The expansion has to be done both in the numerator and in the denominator of the general expression for the average Eq.(3.245). This is a very general problem that forces us to introduce the notion of connected graphs. A generalization of this problem also occurs if we want to compute the free-energy from

$$\ln Z = \ln \left(Tr \left[e^{-\beta H_0} \widehat{U} (\beta, 0) \right] \right) = \ln \left(Z_0 \left\langle \widehat{U} (\beta, 0) \right\rangle_0 \right) \qquad (3.284)$$

$$= \ln \left(\left\langle T_\tau \left[\exp \left(- \int_0^\beta d\tau_1 \widehat{V} (\tau_1) \right) \right] \right\rangle_0 \right) + \ln Z_0 \qquad (3.285)$$

In probability theory this is like computing the cumulant expansion of the characteristic function. Welcome to linked cluster theorems.

These problems are special cases of much more general problems in the theory of random variables which do not even refer to specific Feynman diagrams or to quantum mechanics. The theorems, and their corollary that we prove below, are amongst the most important theorems used in many-body Physics or Statistical Mechanics in general.

Linked cluster theorem for normalized averages

Consider the calculation of

$$\frac{\left\langle e^{-f(\mathbf{x})} A (\mathbf{x}) \right\rangle}{\left\langle e^{-f(\mathbf{x})} \right\rangle} \qquad (3.286)$$

where the expectation $\langle\rangle$ is computed over a multivariate probability distribution function for the variables collectively represented by $\mathbf{x}$. The function $f(\mathbf{x})$ is arbitrary, as is the function $A(\mathbf{x})$. Expanding the exponential, we may write

$$\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle}{\left\langle e^{-f(\mathbf{x})} \right\rangle} = \frac{\sum_{n=0}^{\infty} \frac{1}{n!} \left\langle (-f(\mathbf{x}))^n A(\mathbf{x}) \right\rangle}{\sum_{n=0}^{\infty} \frac{1}{n!} \left\langle (-f(\mathbf{x}))^n \right\rangle} \qquad (3.287)$$

When computing a term of a given order n, such as $\frac{1}{n!} \left\langle (-f(\mathbf{x}))^n A(\mathbf{x}) \right\rangle$, we may always write

$$\frac{1}{n!} \left\langle (-f(\mathbf{x}))^n A(\mathbf{x}) \right\rangle = \sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} \delta_{n,m+\ell} \frac{1}{n!} \frac{n!}{\ell! m!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c \left\langle (-f(\mathbf{x}))^m \right\rangle \qquad (3.288)$$

where the subscript c on the average means that none of the terms in $\left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c$ can be factored into lower order correlation functions, such as for example $\left\langle (-f(\mathbf{x}))^\ell \right\rangle \langle A(\mathbf{x}) \rangle$ or $\left\langle (-f(\mathbf{x}))^{\ell-1} \right\rangle \langle (-f(\mathbf{x})) A(\mathbf{x}) \rangle$ etc... The combinatorial factor corresponds to the number of ways the $(-f(\mathbf{x}))^n$ can be grouped into a group of ℓ terms and a group of $n-\ell$ terms, the $\delta_{n,m+\ell}$ Kronecker delta function ensuring that indeed $m = n - \ell$. Using the last equation in the previous one, the sum over n is now trivially performed with the help of $\delta_{n,m+\ell}$ and one is left with

$$\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle}{\left\langle e^{-f(\mathbf{x})} \right\rangle} = \frac{\sum_{\ell=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{m! \ell!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c \left\langle (-f(\mathbf{x}))^m \right\rangle}{\sum_{n=0}^{\infty} \frac{1}{n!} \left\langle (-f(\mathbf{x}))^n \right\rangle} \qquad (3.289)$$

The numerator can now be factored so as to cancel the denominator which proves the theorem

Theorem 13 *Linked cluster theorem for normalized averages:*

$$\boxed{\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle}{\left\langle e^{-f(\mathbf{x})} \right\rangle} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left\langle (-f(\mathbf{x}))^\ell A(\mathbf{x}) \right\rangle_c = \left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle_c} \qquad (3.290)$$

This result can be applied to our calculation of the Green's function since within the time-ordered product, the exponential may be expanded just as an ordinary exponential, and the quantity which plays the role of $(-f(\mathbf{x}))$, namely $\left(-\int_0^\beta d\tau \widehat{V}(\tau) \right)$ can be moved within the T_τ product without costing any additional minus sign.

Linked cluster theorem for characteristic functions or free energy

We now wish to show the following general theorem for a multivariate probability distribution.

Theorem 14 *Linked cluster theorem (cumulant expansion).*

$$\boxed{\ln \left\langle e^{-f(\mathbf{x})} \right\rangle = \sum_{n=1}^{\infty} \frac{1}{n!} \left\langle (-f(\mathbf{x}))^n \right\rangle_c = \left\langle e^{-f(\mathbf{x})} \right\rangle_c - 1} \qquad (3.291)$$

The proof is inspired by Enz[24]. When $f(\mathbf{x}) = i\mathbf{k} \cdot \mathbf{x}$, the quantity $\left\langle e^{-i\mathbf{k} \cdot \mathbf{x}} \right\rangle$ is called the characteristic function of the probability distribution. It is the generating function for the moments. The quantities on the right-hand side, which as above are connected averages, are usually called *cumulants* in ordinary probability theory and $\ln \left\langle e^{-i\mathbf{k} \cdot \mathbf{x}} \right\rangle$ is the generating function for the cumulant averages.

Proof: To prove the theorem, we introduce first an auxiliary variable λ

$$\frac{\partial}{\partial \lambda} \left\langle e^{-\lambda f(\mathbf{x})} \right\rangle = \left\langle e^{-\lambda f(\mathbf{x})} \left[-f(\mathbf{x}) \right] \right\rangle \tag{3.292}$$

We can apply to the right-hand side the theorem we just proved

$$\left\langle e^{-\lambda f(\mathbf{x})} \left[-f(\mathbf{x}) \right] \right\rangle = \left\langle e^{-\lambda f(\mathbf{x})} \left[-f(\mathbf{x}) \right] \right\rangle_c \left\langle e^{-\lambda f(\mathbf{x})} \right\rangle \tag{3.293}$$

so that

$$\frac{1}{\left\langle e^{-\lambda f(\mathbf{x})} \right\rangle} \frac{\partial}{\partial \lambda} \left\langle e^{-\lambda f(\mathbf{x})} \right\rangle = \left\langle \frac{\partial}{\partial \lambda} e^{-\lambda f(\mathbf{x})} \right\rangle_c. \tag{3.294}$$

Integrating both sides from 0 to 1, we obtain

$$\ln \left\langle e^{-\lambda f(\mathbf{x})} \right\rangle \Big|_0^1 = \left\langle e^{-f(\mathbf{x})} \right\rangle_c - 1 \tag{3.295}$$

QED

Example 15 *It is instructive to check the meaning of the above result explicitly to second order*

$$\ln \left\langle e^{-\lambda f(x)} \right\rangle \approx \ln \left\langle 1 - \lambda f(x) + \frac{1}{2} \left(\lambda f(x) \right)^2 \right\rangle \approx \left(-\left\langle \lambda f(x) \right\rangle + \frac{1}{2} \left\langle \left(\lambda f(x) \right)^2 \right\rangle \right) - \frac{1}{2} \left\langle \lambda f(x) \right\rangle^2 \tag{3.296}$$

$$\left\langle e^{-\lambda f(x)} \right\rangle_c - 1 \approx -\left\langle \lambda f(x) \right\rangle_c + \frac{1}{2} \left\langle \left(\lambda f(x) \right)^2 \right\rangle_c \tag{3.297}$$

so that equating powers of λ, we find as expected,

$$\left\langle \left(f(\mathbf{x}) \right)^2 \right\rangle_c = \left\langle \left(f(\mathbf{x}) \right)^2 \right\rangle - \left\langle f(\mathbf{x}) \right\rangle^2. \tag{3.298}$$

The above results will help us in the calculation of the free energy since we find, as in the first equations of the section on linked cluster theorems,

$$F = -T \ln \left[Z_0 \left\langle T_\tau \left[e^{-\int_0^\beta d\tau \widehat{V}(\tau)} \right] \right\rangle_0 \right] = -T \sum_{n=1}^\infty \frac{1}{n!} \left\langle T_\tau \left[-\int_0^\beta d\tau \widehat{V}(\tau) \right]^n \right\rangle_{0c} -T \ln Z_0 \tag{3.299}$$

$$\boxed{ F = -T \ln Z = -T \left[\left\langle T_\tau \left[e^{-\int_0^\beta d\tau \widehat{V}(\tau)} \right] \right\rangle_{0c} - 1 \right] - T \ln Z_0. } \tag{3.300}$$

the subscript 0 stands for averages with the non-interacting density matrix. The above proof applies to our case because the time-ordered product of an exponential behaves exactly like an ordinary exponential when differentiated, as we know from the differential equation that leads to its definition.

3.7.3 Variational principle and application to Hartree-Fock theory

It is legitimate to ask if there is a one-body Hamiltonian, in other words an effective Hamiltonian with a time-independent potential, whose solution is as close as possible to the true solution. To address this question, we also need to define what we mean by "as close as possible". The answer to both of these queries is provided by the variational principle for thermodynamic systems. We discuss below how Hartree-Fock theory comes out naturally from the variational principle. Also, it is an unavoidable starting point when there is a broken symmetry, as we will discuss more fully in a later chapter.

Thermodynamic variational principle for classical systems

One can base the thermodynamic variational principle for classical systems on the inequality

$$e^x \geq 1 + x \tag{3.301}$$

which is valid for all x, whether $x > 0$, or $x < 0$. This inequality is a convexity inequality which appears obvious when the two functions are plotted. We give two proofs.

Proof 1: e^x is a convex function, *i.e.* $d^2 e^x / d^2 x \geq 0$ for all values of x. At $x = 0$ the functions e^x and $1 + x$ as well as their first derivatives are equal. Since a straight line tangent to a convex curve at a point cannot intersect it anywhere else, the theorem is proven.*QED*

Algebraically, the proof goes as follows.

Proof 2: The equality occurs when $x = 0$. For $x \leq -1$, $e^x \geq 0$ while $1 + x < 0$, hence the inequality is satisfied. For the remaining two intervals, notice that $e^x \geq 1 + x$ is equivalent to

$$\sum_{n=2}^{\infty} \frac{1}{n!} x^n \geq 0. \tag{3.302}$$

For $x \geq 0$, all terms in the sum are positive so the inequality is trivially satisfied. In the only remaining interval, $-1 < x < 0$, the odd powers of x in the infinite-sum version of the inequality are less than zero but the magnitude of each odd power of x is less than the magnitude of the preceding positive power of x, so the inequality (3.302) survives. *QED*

Moving back to our initial purpose, let $\widetilde{H}_0$ be a trial Hamiltonian. Then take $e^{-\beta(\widetilde{H}_0 - \mu N)}/Z_0$ as the trial density matrix corresponding to averages $\langle \rangle_{\widetilde{0}}$. We will use the above inequality Eq.(3.301) to prove that

$$-T \ln Z \leq -T \ln Z_{\widetilde{0}} + \left\langle H - \widetilde{H}_0 \right\rangle_{\widetilde{0}} \tag{3.303}$$

This inequality is a variational principle because $\widetilde{H}_0$ is arbitrary, meaning that we are free to parametrize it and then to minimize with respect to the set of all parameters to find the best one-particle Hamiltonian in our Physically chosen space of Hamiltonians.

Proof Our general result for the free energy in terms of connected terms, Eq.(3.300), is obviously applicable to classical systems. The simplification that occurs there is that since all operators commute, we do not need to worry about the time-ordered product, thus with

$$\widetilde{V} = H - \widetilde{H}_0 \tag{3.304}$$

we have

$$F = -T \ln Z = -T \left[\left\langle e^{-\beta \widetilde{V}} \right\rangle_{\widetilde{0},c} - 1 \right] - T \ln Z_{\widetilde{0}}. \tag{3.305}$$

Using our basic inequality Eq.(3.301) for $e^{-\beta \widetilde{V}}$ we immediately obtain the desired result

$$F \leq -T \left\langle -\beta \widetilde{V} \right\rangle_{\widetilde{0},c} + F_{\widetilde{0}} \tag{3.306}$$

which is just another way of rewriting Eq.(3.303).

It is useful to note that in the language of density matrices, $\rho_0 = e^{-\beta\left(\widetilde{H}_0 - \mu N\right)}/Z_0$ the variational principle Eq.(3.303) reads,

$$\boxed{-T\ln Z \leq Tr\left[\rho_0\left(H - \mu N\right)\right] + T\text{Tr}\left[\rho_0 \ln \rho_0\right]} \qquad (3.307)$$

which looks as if we had the function $(E - \mu N) - TS$ to minimize, quite a satisfactory state of affairs.

Thermodynamic variational principle for quantum systems

For quantum systems, the general result Eq.(3.303) applies but it is more difficult to prove because there is in general no basis that diagonalizes simultaneously each and every term in the expansion of $T_\tau \exp\left[-\int_0^\beta d\tau \widetilde{V}\left(\tau\right)\right]$. If $\widetilde{V}$ was not time dependent, as in the classical case, then matters would be different since $\widetilde{V}^n$ would be diagonal in the same basis as $\widetilde{V}$ and one could apply our inequality Eq.(3.301) in this diagonal basis and prove the theorem. The proof of the variational principle in the quantum case is thus more complicated because of the non-commutation of operators. As far as I know, the proof is due to Feynman [25]. We do not repeat it here.

Application of the variational principle to Hartree-Fock theory

Writing down the most general one-body Hamiltonian with *orthonormal* eigenfunctions left as variational parameters, the above variational principle leads to the usual Hartree-Fock eigenvalue equation. Such a general one-body Hamiltonian would look like

$$\widetilde{H}_0 = \sum_\alpha \int d\mathbf{x} \phi_\alpha^*\left(\mathbf{x}\right)\left(-\frac{\nabla^2}{2m}\right)\phi_\alpha\left(\mathbf{x}\right) c_\alpha^+ c_\alpha \qquad (3.308)$$

with $\phi_\alpha\left(\mathbf{x}\right)$ as variational wave-functions. In the minimization problem, one must add Lagrange multipliers to enforce the constraint that the wave-functions are not only orthogonal but also normalized.

In a translationally invariant system, the one-body wave functions will be plane waves usually, so only the eigenenergies need to be found. This will be done in the following chapter.

It does happen however that symmetry is spontaneously broken. For example, in an anti-ferromagnet the periodicity is halved so that the Hartree-Fock equations will correspond to solving a 2×2 matrix, even when Fourier transforms are used. The matrix becomes larger and larger as we allow more and more general non-translationally invariant states. In the extreme case, the wave functions are different on every site! This is certainly the case in ordinary Chemistry with small molecules or atoms!

3.8   Quantum impurities

An important example that we will encounter in this School is that of a correlated impurity in a bath of non-interacting electrons. Dynamical Mean-Field theory is based on this example. We will only set up the problem without solving it. The Numerical Renormalization Group approach (NRG) and Density Matrix

Renormalization Group are examples of approaches that can be used to solve this problem.

We begin with the Anderson impurity problem. Including the chemical potential we obtain,

$$
\begin{aligned}
K_I &= H_f + H_c + H_{fc} - \mu N & (3.309)\\
H_f &\equiv \sum_\sigma (\varepsilon - \mu) f_{i\sigma}^\dagger f_{i\sigma} + U \left(f_{i\uparrow}^\dagger f_{i\uparrow} \right) \left(f_{i\downarrow}^\dagger f_{i\downarrow} \right) & (3.310)\\
H_c &\equiv \sum_\sigma \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} & (3.311)\\
H_{fc} &\equiv \sum_\sigma \sum_{\mathbf{k}} V_{i\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger f_{i\sigma} + h.c. & (3.312)
\end{aligned}
$$

Note that the sum over $\mathbf{k}$ in the hybridization part of the Hamiltonian H_{fc} basically tells us that it is the local overlap of the conduction band with the impurity that produces the coupling.

Suppose we want to know the properties of the impurities, such as the local density of states. It can be obtained from the Green function

$$
\mathcal{G}_{ff}(\tau) = -\left\langle T_\tau f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle. \tag{3.313}
$$

We will proceed with the equations of motion method. We first write the equations of motion for $c_{\mathbf{k}\sigma}$ and $f_{i\sigma}$

$$
\begin{aligned}
\frac{\partial}{\partial \tau} c_{\mathbf{k}\sigma} &= [H_I, c_{\mathbf{k}\sigma}] & (3.314)\\
&= -(\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma} + V_{i\mathbf{k}} f_{i\sigma} & (3.315)\\
\frac{\partial}{\partial \tau} f_{i\sigma} &= [H_I, f_{i\sigma}] & (3.316)\\
&= -(\varepsilon - \mu) f_{i\sigma} - U f_{i-\sigma}^\dagger f_{i-\sigma} f_{i\sigma} + V_{i\mathbf{k}}^* c_{\mathbf{k}\sigma} & (3.317)
\end{aligned}
$$

Proceeding like our in our earlier derivation of the equations of motion Eq.(3.153) we have

$$
\begin{aligned}
\frac{\partial}{\partial \tau} \mathcal{G}_{ff}(\tau) &= -\delta(\tau) \left\langle \left\{ f_{i\sigma}(\tau), f_{i\sigma}^\dagger \right\} \right\rangle \\
&\quad - \left\langle T_\tau \left(-(\varepsilon - \mu) f_{i\sigma}(\tau) - U f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) + V_{i\mathbf{k}}^* c_{\mathbf{k}\sigma} \right) f_{i\sigma}^\dagger \right\rangle \quad (3.318)\\
&= -\delta(\tau) - (\varepsilon - \mu) \mathcal{G}_{ff}(\tau) + U \left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle + V_{i\mathbf{k}}^* \mathcal{G}_{cf}(\mathbf{k}, i, \tau)
\end{aligned}
$$

where we defined

$$
\mathcal{G}_{cf}(\mathbf{k}, i, \tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle. \tag{3.319}
$$

To eliminate this quantity, we write its equations of motion

$$
\begin{aligned}
\frac{\partial}{\partial \tau} \mathcal{G}_{cf}(\mathbf{k}, i, \tau) &= -\delta(\tau) \left\langle \left\{ c_{\mathbf{k}\sigma}(\tau), f_{i\sigma}^\dagger \right\} \right\rangle \\
&\quad - \left\langle T_\tau \left(-(\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}(\tau) + V_{i\mathbf{k}} f_{i\sigma}(\tau) \right) f_{i\sigma}^\dagger \right\rangle \\
&= -(\varepsilon_{\mathbf{k}} - \mu) \mathcal{G}_{cf}(\mathbf{k}, i, \tau) + V_{i\mathbf{k}} \mathcal{G}_{ff}(\tau) \quad (3.320)
\end{aligned}
$$

It can be solved by going to Matsubara frequencies

$$
\mathcal{G}_{cf}(\mathbf{k}, i, ik_n) = \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{i\mathbf{k}} \mathcal{G}_{ff}(ik_n). \tag{3.321}
$$

Substituting in the equation for $\mathcal{G}_{ff}(ik_n)$ we obtain

$$\left[ik_n - (\varepsilon - \mu) + V_{i\mathbf{k}}^* \frac{1}{ik_n - (\varepsilon_\mathbf{k} - \mu)} V_{i\mathbf{k}} \right] \mathcal{G}_{ff}(ik_n)$$

$$= \quad 1 - U \int_0^\beta d\tau e^{ik_n\tau} \left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle. \qquad (3.322)$$

The equation to be solved has exactly the same structure as we would find for a single impurity except that now the "non-interacting" Green function is

$$\mathcal{G}_{ff}^0(ik_n)^{-1} = ik_n - (\varepsilon - \mu) + V_{i\mathbf{k}}^* \frac{1}{ik_n - (\varepsilon_\mathbf{k} - \mu)} V_{i\mathbf{k}}. \qquad (3.323)$$

This is in fact exactly the non-interacting Green function that we would find with $U = 0$. One can propagate from the impurity site back to the impurity site by going through the bath. One often defines the hybridization function $\Delta_{ff}(ik_n)$ by

$$\Delta_{ff}(ik_n) = V_{i\mathbf{k}}^* \frac{1}{ik_n - (\varepsilon_\mathbf{k} - \mu)} V_{i\mathbf{k}}. \qquad (3.324)$$

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