Mitschrieb zur Vorlesung: Theorie der kondensierten Materie II

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Mitschrieb der Vorlesung Theorie der kondensierten Materie II
von Herrn Prof. Dr. Mirlin und Herrn Dr. Evers im Sommersemester 2008
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Chapter 1

Introduction

Condensed matter are solid states and liquids. As a result of the interaction between particles properties of condensed matter can be very different from the properties of the free particles. One example is an electron in a periodic potential, which we already know from TKM I. It behaves as a quasiparticle with particle spectrum $\varepsilon(k)$ (band structure). This spectrum can be approximated by

$$\varepsilon(k) = \frac{k^2}{2m^*}\,, \tag{1.1}$$

where m^* is an effective mass. In GaAs, for example, the effective mass is given by $m^* = 0,067 m_\mathrm{e}$. For some materials the effective mass is much larger than the mass of the free electron, as for example in $Ce_{1-x}La_xPb_3$. There, it holds that $m^* \approx 10^3 m_\mathrm{e}$. Other properties of the electron, namely spin $s = 1/2$ and charge e remain the same as for the free particle.
Consider the Schrödinger equation with some periodic potential $V(r)$ and energy spectrum E:

$$\left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V(r)\right)\psi(r) = E\psi(r)\,. \tag{1.2}$$

For Coulomb interaction it holds that

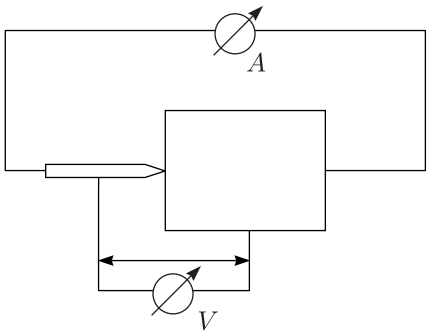
$$\frac{U_\mathrm{int}}{E_\mathrm{kin}} \sim 1\,, \tag{1.3}$$

and it can be $\ll 1$. So, the interaction between electrons is not at all weak.
The interaction leads to modifications and limitations of single-particle picture and therefore new types of excitations. One important example are phonons, the quanta of sound or plasmons, which are collective excitations in an electronic gas. Other excitations are spinons, holons, etc. Let us consider now an electron, which is a fermion with charge e and spin $1/2$. An electronic gas with Coulomb interactions forms plasmons, which are bosons with carge 0 and spin 0. Hence, the excitations have very different properties. How can one describe these excitations physically? The first idea is, to generalize the Schrödinger equation for such a system consiting of N particles:

$$\left[\sum_{i=1}^{N}\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right) + \sum_{i\neq j}^{N} U(|\mathbf{r}_i - \mathbf{r}_j|)\right]\psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N) = E_\alpha\psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_n)\,. \tag{1.4}$$

The realistic number N in a macroscopic system is $\approx 10^{23}$. $\psi_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N;t)$ contains too much information! So, we should reduce the description of our system. What are the physical quantities? These are quantities that

- describe the response of a system on an applied perturbation (as for example electronic or thermal conductivity or tunneling I-V characteristics),



- describe thermodynamic properties (as for example magnetic susceptibility, specific heat).
- Furthermore, it is very important to understand the symmetry of the ground state. The spotlight will be on spontaneous symmetry breaking, which will be essential understand superconductivity, superfluidity and ferromagnetism.
- Properties of elementary particles (quantum numbers and spectra) will be examined.

We now need an appropriate formalism to describe all these properties: the Many-Body Green Function Formalism. This is a field-theoretical description of condensed-matter systems. In practice, this means that one does not use the Schrödinger equation, which is the conventional first quantization, but one uses quantum field theory (second quantization). This approach will allow us to obtain all the information that we will need to calculate the response function, thermodynamical quantities, to understand properties of excitations and to get information about possible instabilities. In most of the cases an exact solution of the problem is not possible; one needs a certain approximation, namely a systematic expansion (perturbation theory) in terms of so-called Feynman diagrams. However, sometimes perturbation theory is not sufficient. Hence, non-perturbative approaches must be applied, such as renormalization group, which is a way to sum all terms in the perturbative expansion to get the most important distributions. Other non-perturbative approaches are bosonization and functional integral methods.

Chapter 2

One-particle Green functions

We start from the Hamiltonian

$$\widehat{H} = -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V(\mathbf{r})\,, \tag{2.1}$$

with the corresponding Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \widehat{H}\psi(\mathbf{r},t)\,. \tag{2.2}$$

No, we define the Green function as

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}_{\mathbf{r}}\right) G(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,, \tag{2.3}$$

where $G(\mathbf{r},t;\mathbf{r}',t')$ is called Green function. In operator language on can write this in the following way:

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}\right)\widehat{G} = \widehat{1}\,. \tag{2.4}$$

Here, one understands $\widehat{G}$ as a kernel of an integral operator. Hence, $\widehat{G}f = g$ is a short-hand notation of

$$\int G(\mathbf{r},t;\mathbf{r}',t')f(\mathbf{r}',t')\,\mathrm{d}\mathbf{r}'\,\mathrm{d}t' = g(\mathbf{r},t)\,. \tag{2.5}$$

The kernel defines, how the integral operator acts on a function $f(x)$:

$$[If](x) = \int \mathrm{d}x'\, I(x,x')f(x')\,. \tag{2.6}$$

Using the notation (2.4) one writes

$$\widehat{G} = \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \widehat{H}\right)^{-1}\,. \tag{2.7}$$

The potential $V(\mathbf{r})$ is t-independent; so the problem is translation invariant in time. Hence, the Green function only depends on the difference of the time variables: $G = G(\mathbf{r},\mathbf{r}',t-t')$. The conjugate variable of the time t in a Fourier transformation is the energy ε:

$$G(\mathbf{r},\mathbf{r}',t-t') = \int \frac{\mathrm{d}\varepsilon}{2\pi}\,\exp\left(-\frac{\mathrm{i}}{\hbar}\varepsilon(t-t')\right) G(\varepsilon;\mathbf{r},\mathbf{r}')\,. \tag{2.8}$$

The Fourier transformation of equation (3.47) is:

$$(\varepsilon - \widehat{H}_{\mathbf{r}})G(\varepsilon;\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\,, \quad \widehat{G} = (\varepsilon - \widehat{H})^{-1}\,. \tag{2.9}$$

The Green function is the propability amplitude of the process $(t'\mathbf{r}') \mapsto (t,\mathbf{r})$.
Let us now consider the analogy to a classical problem, namely the diffusion equation:

$$\left(\frac{\partial}{\partial t} - D\boldsymbol{\nabla}^2\right) P(\mathbf{r},t;\mathbf{r}',t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,. \tag{2.10}$$

The equations (2.9) do not define $\widehat{G}$ uniquely. To demonstrate this, we will consider the simple Hamiltonian of a free particle:

$$\widehat{H} \mapsto \widehat{H}_0 = -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \,. \tag{2.11}$$

The Fourier-transformed equation is given by:

$$\left(\varepsilon + \frac{\hbar^2 \boldsymbol{\nabla}_r^2}{2m}\right) G_0(\varepsilon, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \,. \tag{2.12}$$

A Fourier transformation $r \mapsto p$ leads to

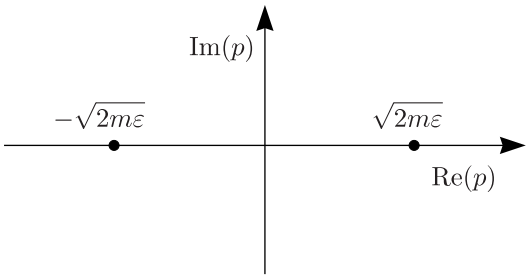
$$G_0(\varepsilon, \mathbf{r} - \mathbf{r}') = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \, G_0(\varepsilon, \mathbf{p}) \exp\left(\frac{\mathrm{i}}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')\right) \,, \tag{2.13}$$

and inserting this one results in:

$$\left(\varepsilon - \frac{p^2}{2m}\right) G_0(\varepsilon, \mathbf{p}) = 1 \Rightarrow G_0(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m}} \,. \tag{2.14}$$

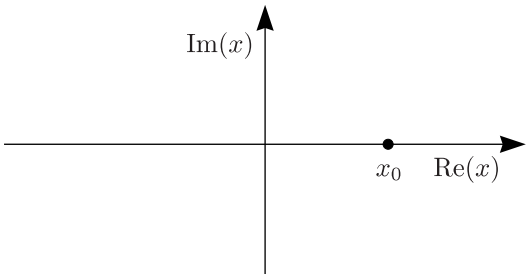
In position space, the Green functions only depends on the difference $\mathbf{r}_1 - \mathbf{r}_2 := \mathbf{r}$:

$$G_0(\varepsilon, \mathbf{r}) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \, \frac{\exp\left(\frac{\mathrm{i}}{\hbar} \mathbf{p} \cdot \mathbf{r}\right)}{\varepsilon - \frac{p^2}{2m}} \,. \tag{2.15}$$



The integrand has got two singularities on the real axis: $p^2 = 2m\varepsilon$.
Be $f(x)$ a smooth function. Consider the integral

$$\int \mathrm{d}x \, \frac{\mathrm{d}x}{x - x_0} f(x) \,. \tag{2.16}$$

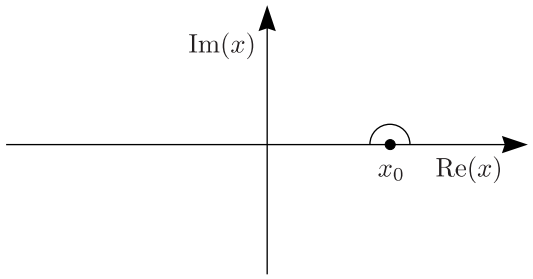


How can this integral be understood? There are different possibilities:

i.) Principal value integral:

$$\mathcal{P} \int \mathrm{d}x \, \frac{f(x)}{x - x_0} = \lim_{\delta \mapsto 0} \left\{ \int_{-\infty}^{x_0 - \delta} \mathrm{d}x \, \frac{f(x)}{x - x_0} + \int_{x_0 + \delta}^{\infty} \mathrm{d}x \, \frac{f(x)}{x - x_0} \right\} \,. \tag{2.17}$$

ii.) Consider x_0 as a complex variable and go around the point x_0 through a half-circle.

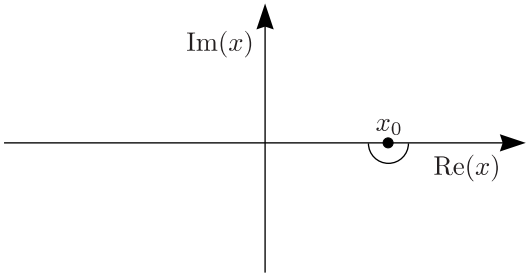


The integrand near the pole has got the value $f(x_0)$. So, one obtains:

ii.) upper complex plane

$$\int \mathrm{d}x \, \frac{f(x)}{x - x_0} - \mathrm{i}\pi f(x_0) \,. \tag{2.18}$$

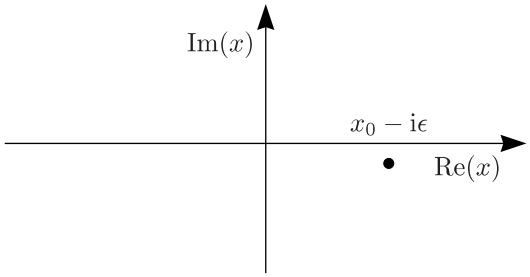
iii.) lower complex plane



$$\int \mathrm{d}x \, \frac{f(x)}{x - x_0} + \mathrm{i}\pi f(x_0) \,. \tag{2.19}$$

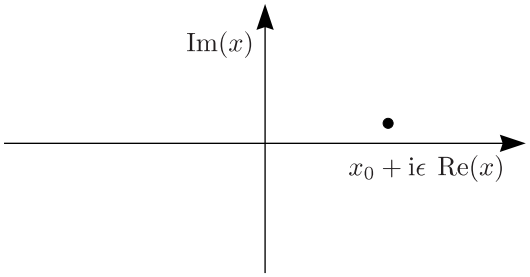
iii.) Shift the pole into the complex plane:

ii.) lower complex plane



$$\int \mathrm{d}x \, \frac{f(x)}{x - x_0 + \mathrm{i}0} \,. \tag{2.20}$$

ii.) upper complex plane



$$\int \mathrm{d}x \, \frac{f(x)}{x - x0 - \mathrm{i}0} \,. \tag{2.21}$$

So, the end result is:

$$\frac{1}{x - x_0 \pm \mathrm{i}0} = \mathcal{P}\frac{1}{x - x_0} \mp \mathrm{i}\pi\delta(x - x_0)\,. \tag{2.22}$$

(i) has got no physical meaning, but (ii) and (iii).

$$\text{(i)} = \frac{\text{(ii)} + \text{(iii)}}{2}\,. \tag{2.23}$$

(ii) corresponds to the so-called retarded Green function:

$$G_0^R(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0}\,, \quad G_0^R(\varepsilon, r) = \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0}\,. \tag{2.24}$$

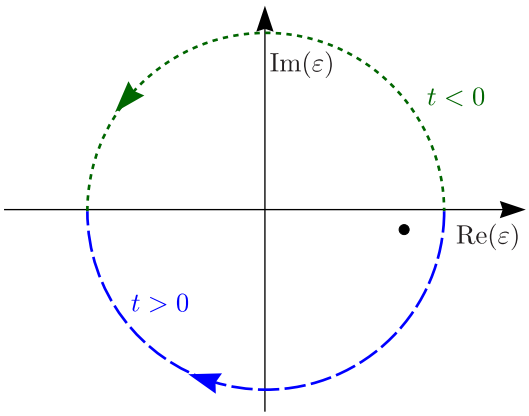
(iii) is the advanced Green function:

$$G_0^A(\varepsilon, \mathbf{p}) = \frac{1}{\varepsilon - \frac{p^2}{2m} - \mathrm{i}0}\,. \tag{2.25}$$

Let us look at the Fourier transforms $\varepsilon \mapsto t$:

$$G_0^R(t, p) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \exp(-\mathrm{i}\varepsilon t) \frac{1}{\varepsilon - \frac{p^2}{2m} + \mathrm{i}0}\,. \tag{2.26}$$

For the calculation of this integral we will use the residue theorem.



For negative times the integration contour must be closed in the upper complex plane and for positive times in the lower complex plane, so that the contour integral along this semi-circle does not contribute (because of the exponential function). The result is:

$$G_0^R(t, p) = \begin{cases} 0 & \text{for} \quad t < 0 \\ -\mathrm{i}\exp\left(-\mathrm{i}\frac{p^2}{2m}t\right) & \text{for} \quad t > 0 \end{cases}\,. \tag{2.27}$$

Since this Green function vanishes for negative times, it is called retarded. For the advanced Green function one obtains:

$$G_0^A(t, p) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \exp(-\mathrm{i}\varepsilon t) \frac{1}{\varepsilon - \frac{p^2}{2m} - \mathrm{i}0} = \begin{cases} \mathrm{i}\exp\left(-\mathrm{i}\frac{p^2}{2m}t\right) & \text{for} \quad t < 0 \\ 0 & \text{for} \quad t > 0 \end{cases}\,. \tag{2.28}$$

The Fourier-transformed with respect to the momentum $\mathbf{p}$ are:

$$G_0^R(t, r) = \theta(t) \frac{1}{(2\pi)^d} \left(\frac{2\pi m}{\mathrm{i}t}\right)^{\frac{d}{2}} \exp\left(-\frac{\mathrm{i}mr^2}{2t}\right)\,, \quad t_1 > t_2\,, \tag{2.29}$$

and

$$G_0^R(t, r) = -\theta(-t) \frac{1}{(2\pi)^d} \left(\frac{2\pi m}{\mathrm{i}t}\right)^{\frac{d}{2}} \exp\left(-\frac{\mathrm{i}mr^2}{2t}\right)\,, \quad t_1 < t_2\,. \tag{2.30}$$

The retarded Green function describes the evolution forwards in time and the advanced Green function the evolution backwards in time. We now want to define Green functions for Hamiltonian with a potential: $\widehat{H} = \widehat{H}_0 + \widehat{V}$.

$$(\varepsilon - \widehat{H})G(\varepsilon, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,. \tag{2.31}$$

$\widehat{H}$ has to a set of eigenfunctions ψ_α to corresponding eigenvalues ε_α. We can write up the following eigenvalue equations:

$$\widehat{H}\psi_\alpha = \varepsilon_\alpha \psi_\alpha\,, \quad H|\psi_\alpha\rangle = \varepsilon_\alpha |\psi_\alpha\rangle\,, \tag{2.32}$$

$$\psi_\alpha^* \widehat{H} = \varepsilon_\alpha \psi_\alpha^*\,, \quad \langle\psi_\alpha| H = \varepsilon_\alpha \langle\psi_\alpha|\,. \tag{2.33}$$

One can use

$$\psi_\alpha^*(\varepsilon - \widehat{H})\widehat{G} = \psi_\alpha^*\,, \tag{2.34}$$

to obtain the following equation:

$$(\varepsilon - \varepsilon_\alpha)\int \mathrm{d}r\, \psi_\alpha^*(\mathbf{r})G(\varepsilon; \mathbf{r}, \mathbf{r}') = \psi_\alpha^*(\mathbf{r}')\,. \tag{2.35}$$

$$G(\varepsilon; \mathbf{r}, \mathbf{r}') = \sum_\alpha \psi_\alpha(\mathbf{r}) A_\alpha \psi_\alpha^*(\mathbf{r}')\,, \quad A_\alpha(\varepsilon - \varepsilon_\alpha) = 1\,. \tag{2.36}$$

$$G^R(\varepsilon; \mathbf{r}, \mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha + \mathrm{i}0}\,. \tag{2.37}$$

$$G^A(\varepsilon, \mathbf{r}, \mathbf{r}') = \sum_\alpha \frac{\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')}{\varepsilon - \varepsilon_\alpha - \mathrm{i}0}\,. \tag{2.38}$$

So, if we write

$$\widehat{H} = \sum_\alpha \varepsilon_\alpha |\alpha\rangle\langle\alpha|\,, \tag{2.39}$$

one obtains:

$$\widehat{G}^{R,A} = \sum_\alpha \frac{|\alpha\rangle\langle\alpha|}{\varepsilon - \varepsilon_\alpha \pm \mathrm{i}0}\,. \tag{2.40}$$

Using

$$\frac{1}{x \pm \mathrm{i}0} = \mathcal{P}\frac{1}{x} \mp \mathrm{i}\pi\delta(x)\,, \tag{2.41}$$

one can derive the spectral weight:

$$A(\varepsilon, \mathbf{r}, \mathbf{r}') = \frac{\mathrm{i}}{2\pi}\left\{G^R(\varepsilon; \mathbf{r}, \mathbf{r}') - G^A(\varepsilon, \mathbf{r}, \mathbf{r}')\right\} = \sum_\alpha \psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}')\delta(\varepsilon - \varepsilon_\alpha)\,. \tag{2.42}$$

It sits a those points of the spectrum, where one has eigenstates. The spectral weight is directly related to the Green functions:

$$G^{R,A}(\varepsilon; \mathbf{r}, \mathbf{r}') = \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon_1\, \frac{A(\varepsilon_1)}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0}\,. \tag{2.43}$$

For $\varepsilon = \varepsilon_\alpha$, A has a δ-peak and $G^{R,A}$ have poles.
Let us now consider the equation for Green functions again:

$$(\varepsilon - \widehat{H})G(\varepsilon; \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,. \tag{2.44}$$

We multiply from the left with G_0 and use $\widehat{H} = \widehat{H}_0 + \widehat{V}$

$$\widehat{G}_0(\varepsilon - \widehat{H})\widehat{G} = \widehat{G}_0\,, \tag{2.45}$$

$$\widehat{G}_0(\varepsilon - \widehat{H}_0)\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}\,, \tag{2.46}$$

and then, we obtain an integral equation for $\widehat{G}$:

$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}\,. \tag{2.47}$$

This is an integral equation for $\widehat{G}$, which is called Dyson equation. We will write it up explicitly:

$$G(\varepsilon, \mathbf{r}, \mathbf{r}') = G_0(\varepsilon, \mathbf{r}, \mathbf{r}') + \int \mathrm{d}r''\, G_0(\mathbf{r}, \mathbf{r}'')V(\mathbf{r}'')G(\mathbf{r}'', \mathbf{r}')\,. \tag{2.48}$$

The equations are the same for retarded and advanced Green functions. These kind of integral equations can be solved by iterations.

- First order approximation:

$$G(\varepsilon, \mathbf{r}, \mathbf{r}') = G_0(\varepsilon, \mathbf{r}, \mathbf{r}')\,, \tag{2.49}$$

- Second order approximation:

$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0\,, \tag{2.50}$$

- n-th order approximation:

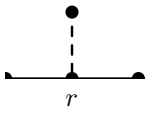
$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0 + \widehat{G}_0\widehat{V}\widehat{G}_0\widehat{V}\widehat{G}_0 + \dots\,. \tag{2.51}$$

$$\widehat{G} = (\varepsilon - \widehat{H})^{-1} = (\varepsilon - \widehat{H}_0 - \widehat{V})^{-1} = (\widehat{G}_0^{-1} - \widehat{V})^{-1}\,. \tag{2.52}$$

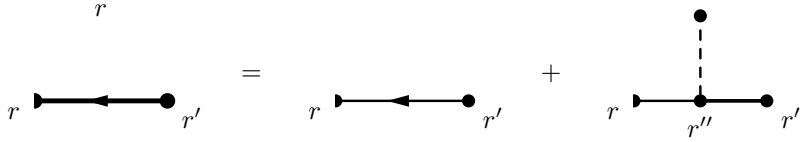
2.1 Diagrams

$G(\varepsilon; \mathbf{r}, \mathbf{r}')$ (2.53)

$G_0(\varepsilon; \mathbf{r}, \mathbf{r}')$ (2.54)



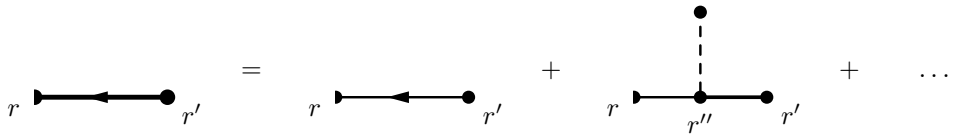
$V(\mathbf{r})$ (2.55)



(2.56a)

$$G = G_0 + G_0VG \tag{2.56b}$$

$$G(\varepsilon; \mathbf{r}, \mathbf{r}') = G_0(\varepsilon; \mathbf{r}, \mathbf{r}') + \int \mathrm{d}r''\, G_0(\varepsilon; \mathbf{r}, \mathbf{r}'')V(\mathbf{r}'')G(\varepsilon; \mathbf{r}'', \mathbf{r}')\,, \tag{2.56c}$$



(2.57a)

$$G = G_0 + G_0VG_0 + \dots \tag{2.57b}$$

Integrations are done over intermediate coordinates.
By Fourier transformation we go to momentum space:

$$G^R(\varepsilon; \mathbf{r}_1, \mathbf{r}_2) = \int \frac{\mathrm{d}^d p_1}{(2\pi)^d} \frac{\mathrm{d}^d p_2}{(2\pi)^d} \exp(\mathrm{i}\mathbf{p}_1 \cdot \mathbf{r}_1 - \mathrm{i}\mathbf{p}_2 \cdot \mathbf{r}_2) G^R(\varepsilon; \mathbf{p}_1, \mathbf{p}_2)\,, \tag{2.58}$$

$$G_0^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) = \underbrace{\frac{1}{\varepsilon - \frac{p_1^2}{2m} + \mathrm{i}0}}_{=G-0^R(\varepsilon;\mathbf{p}_1)} (2\pi)^d \delta(\mathbf{p}_1 - \mathbf{p}_2)\,, \tag{2.59}$$

$$V(\mathbf{r}) = \int \frac{\mathrm{d}^d q}{(2\pi)^d} \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}) V(\mathbf{q})\,, \tag{2.60}$$

Thus, we obtain for the Fourier transform of equation (3.51):

$$\begin{aligned} G^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) = G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) + G_0^R(\varepsilon;\mathbf{p}_1)\int \mathrm{d}r_3 \int \frac{\mathrm{d}^d q}{(2\pi)^d}\frac{\mathrm{d}^d p_3}{(2\pi)^d} \exp(-\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_3)\times \\ \times \exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}_3) V(\mathbf{q}) \exp(\mathrm{i}\mathbf{p}_3\cdot\mathbf{r}_3) G^R(\varepsilon;\mathbf{p}_3,\mathbf{p}_2)\,. \end{aligned} \tag{2.61}$$

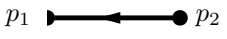
With the representation

$$\int \mathrm{d}r_3 \exp(-\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_3)\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}_3)\exp(\mathrm{i}\mathbf{p}_3\cdot\mathbf{r}_3) = (2\pi)^d\delta(\mathbf{q}+\mathbf{p}_3-\mathbf{p}_1)\,, \tag{2.62}$$

on obtains:

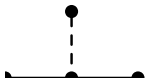
$$\begin{aligned} G^R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2) &= G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) + \int \frac{\mathrm{d}^d p_3}{(2\pi)^d} G_0^R(\varepsilon;\mathbf{p}_1) V(\mathbf{p}_1-\mathbf{p}_3) G^R(\varepsilon;\mathbf{p}_3,\mathbf{p}_2) = \\ &= G_0^R(\varepsilon;\mathbf{p}_1)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2) \\ &\quad + \int \frac{\mathrm{d}^d q}{(2\pi)^d} G_0^R(\varepsilon;\mathbf{p}_1) V(\mathbf{q}) G_0^R(\varepsilon,\mathbf{p}_2)(2\pi)^d\delta(\mathbf{p}_1-\mathbf{q}-\mathbf{p}_2) + \dots\,. \end{aligned} \tag{2.63}$$

2.1.1 Diagrammatics in momentum space

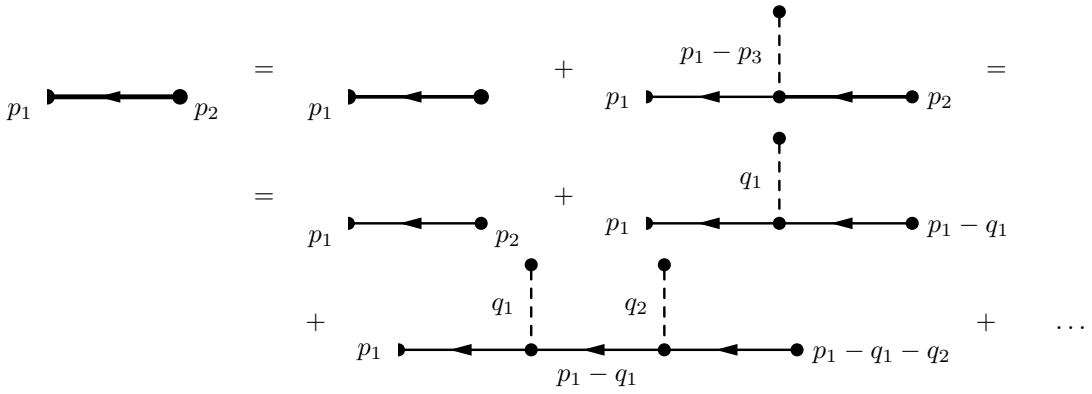


$G_R(\varepsilon;\mathbf{p}_1,\mathbf{p}_2)$ (2.64)

$G_0^R(\varepsilon;\mathbf{p}_1)$ (2.65)

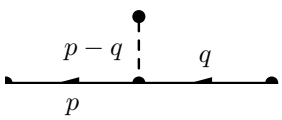


$V(\mathbf{q})$ (2.66)



(2.67)

- At each vertex momentum is conserved.



- $(2\pi)^d\delta(\mathbf{p}_1 - \mathbf{p}_2 - \sum_i \mathbf{q}_i)$
- integrate over all internal momenta: $\int \prod_i \frac{\mathrm{d}^d q_i}{(2\pi)^d}$

2.2 Time-dependent problems

We consider the Hamiltonian (with $\hbar = c = 1$)

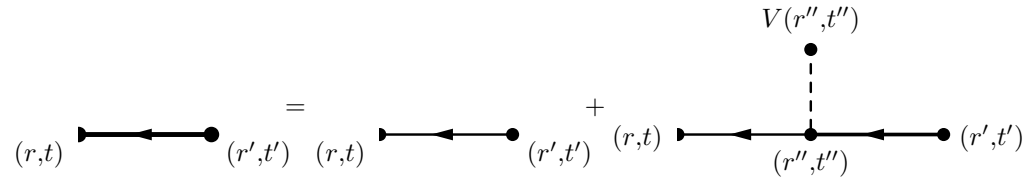
$$\widehat{H} = -\frac{\boldsymbol{\nabla}^2}{2m} + V(\mathbf{r}, t)\,. \tag{2.68}$$

$$\left(\mathrm{i}\frac{\partial}{\partial t} - H(\mathbf{r}, t)\right) G(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\,. \tag{2.69}$$

Because of translation invariance in time, G_0 only depends on time differences. $G(\mathbf{r}, t; \mathbf{r}', t'')$ obeys the original integral equation, whereas has to integrate over intermediate times:

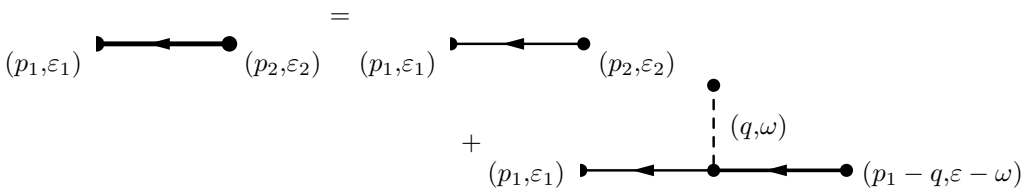
$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r} - \mathbf{r}', t - t') + \int \mathrm{d}r''\mathrm{d}t''\, G_0(\mathbf{r} - \mathbf{r}'', t - t'')V(\mathbf{r}'', t'')G(\mathbf{r}'', t''; \mathbf{r}', t')\,. \tag{2.70}$$

The pictures are the same, but one must understand them differently. If we Fourier transform everything, the energy also will change, because an external potential changes the energy of the physical system.



(2.71)

$$G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \int \frac{\mathrm{d}^d p_1}{(2\pi)^d}\frac{\mathrm{d}^d p_2}{(2\pi)^d}\frac{\mathrm{d}\varepsilon_1}{2\pi}\frac{\mathrm{d}\varepsilon_2}{2\pi}\, \exp(\mathrm{i}\mathbf{p}_1 \cdot \mathbf{r}_1 - \mathrm{i}\mathbf{p}_2 \cdot \mathbf{r}_2 - \mathrm{i}\varepsilon_1 t_1 + \mathrm{i}\varepsilon_2 t_2) G(\mathbf{p}_1, \varepsilon_1; \mathbf{p}_2, \varepsilon_2)\,. \tag{2.72}$$



(2.73)

- energy-momentum conservation in each vertex
- $(2\pi)^d \delta(\mathbf{p}_1 - \mathbf{p}_2 - \sum_i \mathbf{q}_i) \cdot 2\pi\delta(\varepsilon_1 - \varepsilon_2 - \sum_i \omega_i)$
- integrate over internal momenta and energies: $\displaystyle\int \prod_i \frac{\mathrm{d}^d q_i}{(2\pi)^d}\frac{\mathrm{d}\omega_i}{2\pi}$

The first term in the perturbation series is called Born approximation. It is sufficient, if the potential is weak.

Chapter 3

Many-body Green functions

3.1 Second quantization

In order to introduce the many-body Green functions, we will need the formulation of the second quantization. We consider a Hamiltonian of a many-particle problem:

$$\widehat{H} = \sum_{i=1}^{N} \left[-\frac{1}{2m} \boldsymbol{\nabla}_i^2 + V(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i, \mathbf{r}_j) \equiv \widehat{H}_0 + \widehat{V} \,. \tag{3.1}$$

$\widehat{H}_0$ is the sum of one-particles Hamiltonian and $\widehat{V}$ describes the interaction between particles. One has a basis of one-particle states $\psi_k(\mathbf{r})$. Then, one can write any many-body wave function as an expansion in this basis:

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \sum_{k_1, \ldots, k_N} C(k_1, \ldots, k_N; t) \psi_{k_1}(\mathbf{r}_1) \ldots \psi_{k_N}(\mathbf{r}_N) \,, \tag{3.2}$$

where $\{\psi_{k_1}(\mathbf{r}_1), \ldots \psi_{k_N}(\mathbf{r}_N)\}$ are many-body basis states. The coefficients $C(k_1, \ldots, k_N; t)\psi_{k_1}(\mathbf{r}_1)$ should be symmetric for bosons and antisymmetric for fermions to respect the symmetries of the wave functions. Therefore, it is better to choose a more conveniant basis.

3.1.1 Bosons

$$\Phi_{n_1, n_2, n_3, \ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \left(\frac{n_1! n_2! \ldots}{N!} \right)^{\frac{1}{2}} \sum_{\{k_1, k_2, \ldots, k_N\} \Leftrightarrow \{(n_1, n_2, n_3, \ldots)\}} \psi_{k_1}(\mathbf{r}_1) \psi_{k_2}(\mathbf{r}_2) \ldots \psi_{k_N}(\mathbf{r}_N) \,. \tag{3.3}$$

The different states are labeled by the index k. The new basis states are characterized by occupation numbers n_1, n_2, ... n_1, for example, tells us, how many particles are in state with index k_1. One sums over all possibilities in such a way, that $\{k_1, k_2, \ldots, k_N\}$ obeys the occupation number $\{\underbrace{1 \ldots 1}_{n_1} \underbrace{2 \ldots 2}_{n_2} \ldots\}$ (+ all permutations).

Hence, we can write:

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \sum_{n_1, n_2, \ldots} \widetilde{C}(n_1, n_2, \ldots, t) \Phi_{n_1, n_2, \ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \,. \tag{3.4}$$

We will denote $\Phi_{n_1, n_2, \ldots}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ by $|n_1, n_2, \ldots\rangle$. The states are normalized:

$$\langle n_1, n_2, \ldots | n_1', n_2', \ldots \rangle = \delta_{n_1, n_1'} \delta_{n_2, n_2'} \ldots \,. \tag{3.5}$$

The projector

$$\sum_{n_1, n_2, \ldots} |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = \mathbb{1} \,, \tag{3.6}$$

is the unit operator in the space of the states $|n_1, n_2, \ldots\rangle$, the so-called Fock space. The next step is to introduce creation and annihilation operators $a_k^\dagger$ and a_k. It holds that

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} \,, \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0 \,. \tag{3.7}$$

The operators change the occupation numbers of the corresponding states:

$$a_k|n_k\rangle = n_k^{\frac{1}{2}}|n_k-1\rangle\,, \quad a_k^\dagger|n_k\rangle = (n_k+1)^{\frac{1}{2}}|n_k+1\rangle\,, \quad a_k^\dagger a_k|n_k\rangle = n_k|n_k\rangle\,. \tag{3.8}$$

$a_k^\dagger a_k$ is the particle number operator. Any states of these Fock states $|n_1, n_2, \ldots\rangle$ can be written as a result of an application of creation operators on the vacuum state $|0,0,\ldots\rangle \equiv |0\rangle$:

$$|n_1, n_2, \ldots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{(n_k!)^{\frac{1}{2}}}|0\rangle\,. \tag{3.9}$$

We want to write the Hamiltonian in terms of creation and annihilation operators. So, let us consider:

$$\sum_i \widehat{H}_0(\mathbf{r}_i)\Phi_{n_1,n_2,n_3,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\,, \tag{3.10}$$

With

$$\widehat{H}_0\psi_k = \sum_{k'}(H_0)_{kk'}\psi_{k'}\,, \quad \text{with } (H_0)_{k'k} = \langle k'|H_0|k\rangle = \int \mathrm{d}^d r\, \psi_{k'}^*(\mathbf{r})\widehat{H}_0(\mathbf{r})\psi_k(\mathbf{r})\,, \tag{3.11}$$

one obtains:

$$\sum_k n_k(H_0)_{kk}\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) + \sum_{k\neq k'} n_k^{\frac{1}{2}}(n_{k'}+1)^{\frac{1}{2}}(H_0)_{k'k}\Phi_{n_1,n_2,\ldots,n_k-1,\ldots,n_{k'}+1,\ldots}\,. \tag{3.12}$$

Now, one can write the Hamiltonian in the second quantization language as follows:

$$= \sum_{k,k'}(H_0)_{k'k}a_{k'}^\dagger a_k|n_1,n_2,\ldots\rangle \tag{3.13}$$

$$\sum_i \widehat{H}_0(\mathbf{r}_i) \Leftrightarrow \sum_{k,k'}(H_0)_{k'k}a_{k'}^\dagger a_k\,. \tag{3.14}$$

Exactly in the same way one can consider the interaction part of the Hamiltonian. The calculation works analogously and one obtains:

$$\frac{1}{2}\sum_{i\neq j}V(\mathbf{r}_i,\mathbf{r}_j) \Leftrightarrow \frac{1}{2}\sum_{k,l,m,n} V_{kl;mn}a_k^\dagger a_l^\dagger a_m a_n\,, \tag{3.15}$$

where it holds that

$$V_{kl;mn} = \int \mathrm{d}r\,\mathrm{d}r'\,\psi_k^*(\mathbf{r})\psi_l^*(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\psi_m(\mathbf{r})\psi_n(\mathbf{r}')\,. \tag{3.16}$$

Hence, the full Hamiltonian can be equivalently written as follows:

$$\widehat{H} \Leftrightarrow \sum_{k,l}(H_0)_{kl}a_k^\dagger a_l + \frac{1}{2}\sum_{k,l,m,n} V_{kl;mn}a_k^\dagger a_l^\dagger a_m a_n\,. \tag{3.17}$$

That is, how operators are translated from first to second quantization.

3.1.2 Fermions

For fermions the occupation number is either zero or one: $n_k = 0,\, 1$. That respects the Pauli principle.

$$\begin{aligned}\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) &= \frac{1}{(N!)^{\frac{1}{2}}}\sum_{\substack{\text{Permutations}\\ \text{of } \{k_1,\ldots,k_N\}}}(-1)^P\psi_{k_{p_1}}(\mathbf{r}_1)\ldots\psi_{k_{p_N}}(\mathbf{r}_N) = \\ &= \frac{1}{(N!)^{\frac{1}{2}}}\begin{vmatrix}\psi_{k_1}(\mathbf{r}_1) & \ldots & \psi_{k_1}(\mathbf{r}_N)\\ \vdots & \ddots & \vdots\\ \psi_{k_N}(\mathbf{r}_1) & \ldots & \psi_{k_N}(\mathbf{r}_N)\end{vmatrix}\,.\end{aligned} \tag{3.18}$$

The above determinant is called Slater determinant. The creation and annihilation operators satisfy anti-commutation relations:

$$\{a_k, a_{k'}^\dagger\} = \delta_{kk'}\,, \quad \{a_k, a_{k'}\} = \{a_k^\dagger, a_{k'}^\dagger\} = 0\,. \tag{3.19}$$

Furthermore, it holds that

$$a^\dagger|0\rangle = 1\rangle\,, \quad a|1\rangle = |0\rangle\,, \quad a^\dagger|1\rangle = 0\,, \quad a|0\rangle = 0\,, \quad a_k^\dagger a_k = n_k\,. \tag{3.20}$$

Many-body states are labeled by occupation numbers and are created by acting creation operators on the vacuum state:

$$|n_1, n_2, \ldots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\ldots|0\rangle\,, \quad \text{with } |0\rangle \equiv |0, 0, \ldots\rangle\,. \tag{3.21}$$

The Hamiltonian has the same structure as for bosons.

3.2 Field operators

We will go from the basis of single-particle states ψ_k to the basis labeled by the spatial coordinate $\mathbf{r}$. The field operator is given by

$$\widehat{\Psi}(\mathbf{r}) = \sum_k a_k \psi_k(\mathbf{r})\,. \tag{3.22}$$

$\widehat{\Psi}(\mathbf{r})$ is an operator in the Fock space as it is a linear combination of annihilation operators a_k. The $\psi_k(\mathbf{r})$ serve as coefficients. In the same way one defines

$$\widehat{\Psi}(\mathbf{r}) = \sum_k \psi_k^*(\mathbf{r}) a_k^\dagger\,. \tag{3.23}$$

We calculate the commutation relations of these new operators. Firstly, bosons shall be considered:

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')] = \sum_{k,k'} \psi_k(\mathbf{r})\psi_{k'}^*(\mathbf{r}')[a_k, a_{k'}^\dagger] = \sum_k \psi_k(\mathbf{r})\psi_k^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\,, \tag{3.24}$$

$$\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}') = 0 = [\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]\,. \tag{3.25}$$

For fermions one obtains:

$$\{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}')\,, \quad \{\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}(\mathbf{r}')\} = \{\widehat{\Psi}^\dagger(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\} = 0\,. \tag{3.26}$$

One can put the above formulas together in the form

$$[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]_\mp \equiv \widehat{\psi}(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}') \mp \widehat{\Psi}^\dagger(\mathbf{r}')\widehat{\Psi}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')\,, \tag{3.27}$$

where the upper sign is reserved for bosons and the lower one for fermions. Let us now write the Hamiltonian in terms of the field operators:

$$\widehat{H} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r}) H_0(\mathbf{r}) \widehat{\Psi}(\mathbf{r}) + \frac{1}{2}\int \mathrm{d}r\, \mathrm{d}r'\, \widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}')V(\mathbf{r}, \mathbf{r}')\widehat{\Psi}(\mathbf{r}')\widehat{\Psi}(\mathbf{r})\,. \tag{3.28}$$

Up to now we have neglected the existence of spin. So, we now map $\mathbf{r} \mapsto \mathbf{r}, \sigma$ and then it holds thats

$$[\widehat{\Psi}_\sigma(\mathbf{r}), \widehat{\Psi}_{\sigma'}^\dagger(\mathbf{r}')]_\mp = \delta(\mathbf{r} - \mathbf{r}')\delta_{\sigma\sigma'}\,. \tag{3.29}$$

The density operator $\varrho_{\mathbf{r}_0}$ tells us, what the density of particles at a given point $\mathbf{r}_0$ is:

$$\varrho_{\mathbf{r}_0} = \sum_{i=1}^N \delta(\mathbf{r}_i - \mathbf{r}_0) = \sum_{i=1}^N \varrho_{\mathbf{r}_0}(\mathbf{r}_i)\,, \quad \text{with } \varrho_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r}_0 - \mathbf{r})\,. \tag{3.30}$$

In the language of second quantization the density operator is given by

$$\widehat{\varrho}_{\mathbf{r}_0} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r})\delta(\mathbf{r}_0 - \mathbf{r})\widehat{\Psi}(\mathbf{r}) = \widehat{\Psi}^\dagger(\mathbf{r}_0)\widehat{\Psi}(\mathbf{r}_0)\,. \tag{3.31}$$

The total particle operator is defined by

$$\widehat{N} = \int \mathrm{d}r\, \widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}(\mathbf{r})\,, \tag{3.32}$$

and tells us, how many particle there are in the considered system. From $\widehat{H}' = \widehat{H} - \mu\widehat{N}$ one realizes that it holds

$$H_0(\mathbf{r}) \mapsto -\frac{1}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{r}) - \mu\,, \tag{3.33}$$

where μ is the chemical potential.

$$\exp\left(-\frac{E_n - \mu N_n}{k_B T}\right) \equiv \exp\left(-\frac{E'_n}{k_B T}\right)\,. \tag{3.34}$$

At $T = 0$ the system is in the ground state with the minimal energy E'_0. The ground state will be changed by the chemical potential. If one considers for example a metal, it will make sense not to define the ground state of the metal as the state without any electron.

3.3 Schrödinger versus Heisenberg representations

The standard picture in quantum mechanics is the Schrödinger picture, in which the states are time dependent and obey the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}|\phi(t)\rangle_S = \widehat{H}|\phi(t)\rangle_S\,. \tag{3.35}$$

The Hamilton operator $\widehat{H}$ is t-independent, if there is no external t-dependence. The Schrödinger equation yields the unitary time evolution of the states:

$$|\phi(t)\rangle_S = \exp(-\mathrm{i}\widehat{H}t)|\phi(0)\rangle_S\,. \tag{3.36}$$

In the Heisenberg picture the wave function is t-independent: $|\phi\rangle = \phi(0)\rangle$. The pay for this is that the t-dependence is shifted from the wave functions to operators:

$$O_H(t) = \exp(\mathrm{i}\widehat{H}t)O_S\exp(-\mathrm{i}\widehat{H}t)\,, \tag{3.37}$$

where $O_H(t)$ is the operator in the Heisenberg picture and O_S the operator in the Schrödinger picture. $O_H(t)$ obeys the Heisenberg equation

$$\mathrm{i}\frac{\partial}{\partial t}O_H(t) = [O_H(t), \widehat{H}]\,. \tag{3.38}$$

These two pictures are equivalent by computing matrix elements:

$$\langle\phi_1(t)|O|\phi_2(t)\rangle_S = \langle\phi_1|O(t)|\phi_2\rangle_H\,. \tag{3.39}$$

Anyway it holds that

$$\widehat{H}_S = \widehat{H}_H(t)\,. \tag{3.40}$$

$$\begin{aligned}\widehat{H}(t) &= \exp(\mathrm{i}\widehat{H}t)\left\{\int \mathrm{d}r\,\widehat{\Psi}^\dagger H_0\widehat{\Psi} + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\,\widehat{\Psi}^\dagger(\mathbf{r})\widehat{\Psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}')\widehat{\Psi}(\mathbf{r})\right\}\exp(-\mathrm{i}\widehat{H}t) = \\ &= \int \mathrm{d}r\,\widehat{\Psi}^\dagger(\mathbf{r},t)H_0(\mathbf{r})\Psi^\dagger(\mathbf{r},t) + \frac{1}{2}\iint \mathrm{d}r\,\mathrm{d}r'\,\widehat{\Psi}^\dagger(\mathbf{r},t)\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)\end{aligned} \tag{3.41}$$

For Heisenberg operators the commutator

$$[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t')]_\mp\,, \tag{3.42}$$

is complicated, in general. (It is related to Green functions.) However, at the same times $t = t'$ the commutator becomes relatively simple:

$$\begin{aligned}[\widehat{\Psi}(\mathbf{r},t), \widehat{\Psi}^\dagger(\mathbf{r}',t)] &= [\exp(\mathrm{i}Ht)\widehat{\Psi}(\mathbf{r})\exp(-\mathrm{i}Ht), \exp(\mathrm{i}Ht)\widehat{\Psi}(\mathbf{r}')\exp(-\mathrm{i}Ht)] = \\ &= \exp(\mathrm{i}Ht)[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')]\exp(-\mathrm{i}Ht) = \delta(\mathbf{r} - \mathbf{r}')\,.\end{aligned} \tag{3.43}$$

The nontrivial contribution will come from different times.

3.3.1 Schrödinger equation for $\widehat{\Psi}(\mathbf{r},t)$

$$\mathrm{i}\frac{\partial}{\partial t}\widehat{\Psi}(\mathbf{r},t)=[\widehat{\Psi}(\mathbf{r},t),\widehat{H}]=\left(-\frac{\boldsymbol{\nabla}^2}{2m}+V(\mathbf{r})-\mu\right)\widehat{\Psi}(\mathbf{r},t)+\int \mathrm{d}r'\,\widehat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\widehat{\Psi}(\mathbf{r}',t)\widehat{\Psi}(\mathbf{r},t)\,. \tag{3.44}$$

This equation is nonlinear, so the field operators behave in a nontrivial way.

3.4 Green function

We define

$$G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=-\mathrm{i}\langle\phi_0|T\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)|\phi_0\rangle\,, \tag{3.45}$$

where $|\phi_0\rangle$ is the exact ground state. $TO_1(t_1)O_2(t_2)\dots O_n(t_n)$ is the chronological product, which is defined in the following way:

$$TO_1(t_1)O_2(t_2)\dots O_n(t_n)=O_{i_1}(t_{i_1})O_{i_2}(t_{i_2})\dots O_{i_n}(t_{i_n})\times\begin{cases}1 & \text{for bosons}\\ (-1)^\Sigma & \text{for fermions}\end{cases},\quad \text{for } t_{i_1}>t_{i_2}>\ldots>t_{i_n}\,. \tag{3.46}$$

T is the time ordering operator, which orders the different times such that they increase from right to left. So, the Green function is given by:

$$\begin{aligned}G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)&=\begin{cases}-\mathrm{i}\langle\phi_0|\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)|\phi_0\rangle & \text{for}\quad t_1>t_2\\ \mp\mathrm{i}\langle\phi_0|\widehat{\Psi}^\dagger_{\sigma_2}(\mathbf{r}_2,t_2)\widehat{\Psi}_{\sigma_1}(\mathbf{r}_1,t_1)|\phi_0\rangle & \text{for}\quad t_2>t_1\end{cases}\equiv\\ &\equiv-\mathrm{i}\left\{\theta(t_1-t_2)\langle\phi_0|\psi_1\psi_2^\dagger|\phi_0\rangle\mp\theta(t_2-t_1)\langle\phi_0\psi_2^\dagger\psi_1|\phi_0\rangle\right\}\end{aligned} \tag{3.47}$$

- Under the assumption, that spin-symmetry is not broken, it holds that

$$G_{\sigma_1\sigma_2}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=\delta_{\sigma_1\sigma_2}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)\,. \tag{3.48}$$

- If there is translational invariance in coordinate space, then it is conveniant to go to momentum space by Fourier transformation:

$$G(\mathbf{p}_1,t_1;\mathbf{p}_2,t_2)=-\mathrm{i}\langle\phi_0|T\widehat{\psi}(\mathbf{p}_1,t_1)\widehat{\psi}^\dagger(\mathbf{p}_2,t_2)|\phi_0\rangle\xrightarrow{\text{trans. invariance}}G(\mathbf{p}_1;t_1,t_2)\cdot(2\pi)^d\delta(\mathbf{p}_1-\mathbf{p}_2)\,. \tag{3.49}$$

- If there is translational invariance with respect to the time, then it is conveniant to go to energy space by Fourier transformation:

$$G(\mathbf{p}_1,\mathbf{p}_2,\omega_1)\cdot(2\pi)^d\delta(\omega_1-\omega_2)\,. \tag{3.50}$$

3.5 Non-interacting fermions

In this case the Hamiltonian is given by $H=H_0$, so it holds that $V=0$. The Green function $G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ was defined as a solution of the following equation:

$$(\mathrm{i}\partial_{t_1}-H_0(\mathbf{r}_1))G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=\delta(\mathbf{r}_1-\mathbf{r}_2,t_1-t_2)\,, \tag{3.51}$$

with

$$H_0(\mathbf{r}_1)=-\frac{\boldsymbol{\nabla}^2}{2m}+V(r)-\mu\,. \tag{3.52}$$

We want to proof that (3.47) obeys (3.51). By using

$$(\mathrm{i}\partial_t-H_0)\widehat{\psi}(\mathbf{r},t)=0\,, \tag{3.53}$$

we obtain:

$$\begin{aligned}(\mathrm{i}\partial_{t_1}-H_0(\mathbf{r}_1)G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)&=\delta(t_1-t_2)\mathrm{i}(-\mathrm{i})\langle\phi_0|\psi(\mathbf{r}_1,t_1)\psi^\dagger(\mathbf{r}_2,t_2)+\psi^\dagger(\mathbf{r}_2,t_1)\psi(\mathbf{r}_1,t_1)|\phi_0\rangle=\\ &=\delta(t_1-t_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\,,\end{aligned} \tag{3.54}$$

so it holds that

$$(\mathrm{i}\partial_t - H)G = \mathbb{1}\,. \tag{3.55}$$

We use

$$H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}\,, \tag{3.56}$$

with

$$\varepsilon_{\mathbf{p}} = \frac{p^2}{2m} - \mu\,, \tag{3.57}$$

and

$$\widehat{\psi}^\dagger(\mathbf{r}) = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}} \frac{\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r})}{\sqrt{V}}\,, \quad \widehat{\psi}(\mathbf{r}) = \sum_{\mathbf{p}} a_{\mathbf{p}} \frac{\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})}{\sqrt{V}}\,. \tag{3.58}$$

For the Green function we need the operators in the Heisenberg picture. By using

$$[a^\dagger_{\mathbf{p}} a_{\mathbf{p}}, a^\dagger_{\mathbf{p}}] = a^\dagger_{\mathbf{p}}\,, \quad a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \cdot a^\dagger_{\mathbf{p}} = a^\dagger_{\mathbf{p}}(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + 1)\,, \tag{3.59}$$

and therefore

$$\exp(\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) a^\dagger_{\mathbf{p}} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) = a^\dagger_{\mathbf{p}} \exp(\mathrm{i}\varepsilon_{\mathbf{p}}(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + 1)t) \exp(-\mathrm{i}\varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} t) = a^\dagger_{\mathbf{p}} \exp(\mathrm{i}\varepsilon_{\mathbf{p}} t)\,, \tag{3.60}$$

and we obtain:

$$\psi^\dagger(\mathbf{r}, t) = \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}} \frac{\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r} + \mathrm{i}\varepsilon_{\mathbf{p}} t)}{\sqrt{V}}\,, \quad \psi(\mathbf{r}, t) = \sum_{\mathbf{p}} a_{\mathbf{p}} \frac{\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}} t)}{\sqrt{V}}\,. \tag{3.61}$$

With all states up to the Fermi level filled

$$|\phi_0\rangle = \prod_{\mathbf{p}<\mathbf{p}_F} a^\dagger_{\mathbf{p}} |0\rangle\,, \tag{3.62}$$

the Green function (for $t_1 > t_2$) is given by:

$$\begin{aligned} G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \frac{1}{V} \sum_{\mathbf{p}_1, \mathbf{p}_2} (-\mathrm{i}) \exp(-\mathrm{i}\varepsilon_{\mathbf{p}_1} t_1 + \mathrm{i}\varepsilon_{\mathbf{p}_2} t_2 + \mathrm{i}\mathbf{p}_1\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\mathbf{r}_2) \underbrace{\langle \phi_0 a_{\mathbf{p}_1} a^\dagger_{\mathbf{p}_2} |\phi_0\rangle}_{=\delta_{\mathbf{p}_1\mathbf{p}_2}} \theta(\mathbf{p}_1 - \mathbf{p}_F) = \\ &= -\mathrm{i}\frac{1}{V} \sum_{\mathbf{p}} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}}(t_1 - t_2) + \mathrm{o}\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_2)) \theta(\mathbf{p} - \mathbf{p}_F)\,, \end{aligned} \tag{3.63}$$

and for $t_1 < t_2$:

$$\begin{aligned} G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \frac{1}{V} \sum_{\mathbf{p}_1, \mathbf{p}_2} (\mathrm{i}) \exp(-\mathrm{i}\varepsilon_{\mathbf{p}_1} t_1 + \mathrm{i}\varepsilon_{\mathbf{p}_2} t_2 + \mathrm{i}\mathbf{p}_1\mathbf{r}_1 - \mathrm{i}\mathbf{p}_2\mathbf{r}_2) \underbrace{\langle \phi_0 a^\dagger_{\mathbf{p}_2} a_{\mathbf{p}_1} |\phi_0\rangle}_{=\delta_{\mathbf{p}_1\mathbf{p}_2}} \theta(\mathbf{p}_F - \mathbf{p}_1) = \\ &= \mathrm{i}\frac{1}{V} \sum_{\mathbf{p}} \exp(-\mathrm{i}\varepsilon_{\mathbf{p}}(t_1 - t_2) + \mathrm{i}\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_2)) \theta(\mathbf{p}_F - \mathbf{p})\,, \end{aligned} \tag{3.64}$$

and finally, one obtains for the Fourier transform:

$$G(\mathbf{p}, t) = \begin{cases} -\mathrm{i}\exp(-\mathrm{i}\varepsilon_{\mathbf{p}} t)\theta(\mathbf{p} - \mathbf{p}_F) & \text{for} \quad t > 0 \\ \mathrm{i}\exp(-\mathrm{i}\varepsilon_{\mathbf{p}} t)\theta(\mathbf{p}_F - \mathbf{p}) & \text{for} \quad t < 0 \end{cases}\,. \tag{3.65}$$

We transform to the energy space:

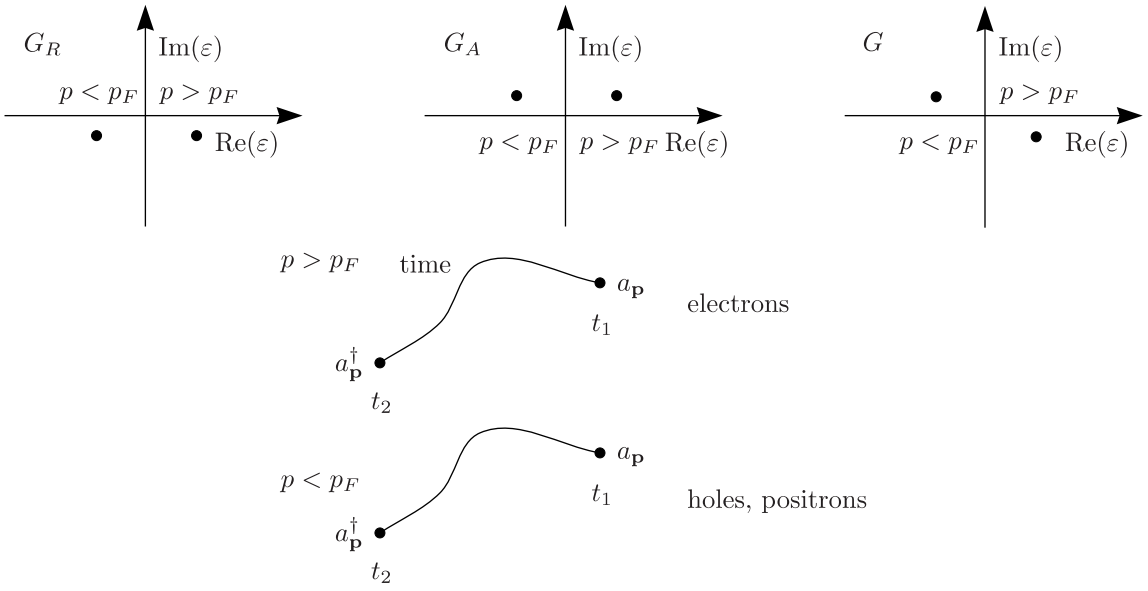
$$\begin{aligned} G(\mathbf{p}, \varepsilon) &= \int \mathrm{d}t\, \exp(\mathrm{i}\varepsilon t) G(\mathbf{p}, t) = \\ &= -\mathrm{i}\left\{ \theta(\mathbf{p} - \mathbf{p}_F) \int_0^\infty \exp(\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}})t - 0t) - \theta(\mathbf{p}_F - \mathbf{p}) \int_{-\infty}^0 \mathrm{d}t\, \exp(\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}})t + 0t) \right\} = \\ &= -\mathrm{i}\left[\theta(\mathbf{p} - \mathbf{p}_F) \frac{1}{-\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}}) + 0} - \theta(\mathbf{p}_F - \mathbf{p}) \frac{1}{\mathrm{i}(\varepsilon - \varepsilon_{\mathbf{p}}) + 0} \right] = \\ &= \frac{\theta(\mathbf{p} - \mathbf{p}_F)}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0} + \frac{\theta(\mathbf{p}_F - \mathbf{p})}{\varepsilon - \varepsilon_{\mathbf{p}} - \mathrm{i}0} \equiv \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}\,\mathrm{sign}(\mathbf{p} - \mathbf{p}_F)}\,. \end{aligned} \tag{3.66}$$

Let us look at the singularity structure of

$$G_R = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0}\,, \tag{3.67}$$

and

$$G_A = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} - \mathrm{i}0}\,, \tag{3.68}$$



The particles, which look like propagating back in time, are holes! We can also write

$$G^R(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = -\mathrm{i}\langle\phi_0|\{\widehat{\psi}(\mathbf{r}_1, t_1), \widehat{\psi}(\mathbf{r}_2, t_2)\}|\phi_0\rangle\theta(t_1 - t_2)\,, \tag{3.69}$$

and

$$G^A(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \mathrm{i}\langle\phi_0|\{\widehat{\psi}(\mathbf{r}_1, t_1), \widehat{\psi}(\mathbf{r}_2, t_2)\}|\phi_0\rangle\theta(t_2 - t_1)\,. \tag{3.70}$$

3.6 Spectral representation of Green functions

This goes back to Lehmann.

3.6.1 Fermions

We start from the general definition (because of translational invariance we set $t_1 = t$ and $t_2 = 0$):

$$\mathrm{i}G(\mathbf{r}, \mathbf{r}', t) = \langle\phi_0|T\widehat{\phi}(\mathbf{r}, t)\widehat{\psi}^\dagger(\mathbf{r}', 0)|\phi_0\rangle - \theta(-t)\langle\phi_0|\widehat{\psi}^\dagger(\mathbf{r}', 0)\widehat{\psi}(, t)|\phi_0\rangle\,. \tag{3.71}$$

The Hamiltonian H' obeys the eigenvalue equation

$$H'|\phi_n^{(N)}\rangle = E'_n|\phi_n^{(N)}\rangle\,, \tag{3.72}$$

with the energy

$$E'_n = E_n - \mu N\,, \tag{3.73}$$

where the eigenstates $|\phi_n^{(N)}$ are labeled by n and (N) stands for the number of particles. We insert

$$\sum_{n,N} |\phi_n^{(N)}\rangle\langle\phi_n^{(N)}| = \mathbb{1}\,, \tag{3.74}$$

and then following matrix elements appear:

$$\begin{aligned}\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r}, t)|\phi_n^{(N)}\rangle &= \langle\phi_m^{(N-1)}\exp(\mathrm{i}H't)\widehat{\psi}(\mathbf{r})\exp(-\mathrm{i}H't)|\phi_n^{(N)}\rangle = \exp(\mathrm{i}(E'_m - E'_n)t)\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r})|\phi_n^{(N)}\rangle = \\ &= \exp(\mathrm{i}(E_m^{(N-1)} - E_n^{(N)} + \mu)t)\langle\phi_m^{(N-1)}\widehat{\psi}(\mathbf{r})|\phi_n^{(N)}\rangle\,.\end{aligned} \tag{3.75}$$

So, we have pulled out the time dependence of the matrix element. $|\phi_0^{(N)}\rangle$ be the ground state; hence, N is the number of particles in the ground state. Let us now calculate the Green function:

$$\begin{aligned}
\mathrm{i}G(\mathbf{r},\mathbf{r}',t) &= \theta(t)\sum_m \langle\phi_0^{(N)}|\widehat{\psi}(\mathbf{r},t)|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\psi}^\dagger(\mathbf{r}',0)|\phi_0^{(N)}\rangle \\
&\quad - \theta(-t)\sum_m \langle\phi_0^{(N)}|\widehat{\psi}^\dagger(\mathbf{r}',0)|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r},t)|\phi_0^{(N)}\rangle = \\
&= \theta(t)\sum_m \exp(\mathrm{i}(E_0^{(N)} - E_m^{(N+1)} + \mu)t)\langle\phi_0^{(N)}|\widehat{\psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}\widehat{\psi}(\mathbf{r}')^\dagger|\phi_0^{(N)}\rangle \\
&\quad - \theta(-t)\sum_m \exp(\mathrm{i}(E_m^{(N-1)} - E_0^{(N)} + \mu)t)\langle\phi_0^{(N)}|\widehat{\psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r})|\phi_0^{(N)}\rangle\,.
\end{aligned} \tag{3.76}$$

We go to energy space by Fourier transformation, because all the time dependence is in the exponential factors:

$$\begin{aligned}
G(\mathbf{r},\mathbf{r}',\varepsilon) = \sum_m \Bigg\{ &\frac{\langle\phi_0^{(N)}|\widehat{\psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\psi}^\dagger(\mathbf{r}')|\phi_0^{(N)}\rangle}{\varepsilon + E_0^{(N)} - E_m^{(N+1)} + \mu + \mathrm{i}0} \\
&+ \frac{\langle\phi_0^{(N)}|\widehat{\psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r})|\phi_0^{(N)}\rangle}{\varepsilon + E_m^{(N-1)} - E_0^{(N)} + \mu - \mathrm{i}0} \Bigg\}\,.
\end{aligned} \tag{3.77}$$

Since E_0 is the ground state, it holds that $E_0' < E_m'$. $E_m^{(N+1)} - E_0^{(N)} \equiv \varepsilon_m^{(+)} > \mu$ is the energy of a particle-like excitation. It should hold that $\varepsilon_m^{(+)} > \mu$. $E_0^{(N)} - E_m^{(N-1)} \equiv \varepsilon_m^{(-)} < \mu$ is the energy of a hole-like excitation. Here, it should hold that $\varepsilon_m^{(-)} < \mu$.
Spectral weight:

$$\begin{aligned}
A(\mathbf{r},\mathbf{r}';\varepsilon_1) = \sum_m \Big\{ &\langle\phi_0^{(N)}|\widehat{\psi}(\mathbf{r})|\phi_m^{(N+1)}\rangle\langle\phi_m^{(N+1)}|\widehat{\psi}^\dagger(\mathbf{r}')|\phi_0^{(N)}\rangle\delta(\varepsilon_1 - \varepsilon_m^{(+)} + \mu) \\
&+\langle\phi_0^{(N)}|\widehat{\psi}^\dagger(\mathbf{r}')|\phi_m^{(N-1)}\rangle\langle\phi_m^{(N-1)}|\widehat{\psi}(\mathbf{r})|\phi_0^{(N)}\rangle\delta(\varepsilon_1 - \varepsilon_m^{(-)} + \mu)\Big\} \equiv \\
\equiv A^{(+)}(\varepsilon_1;\mathbf{r},\mathbf{r}') + A^{(-)}(\varepsilon_1;\mathbf{r},\mathbf{r}')
\end{aligned} \tag{3.78}$$

$A^{(+)}$ is $\neq 0$ only for $\varepsilon_1 > 0$ und $A^{(-)}$ ist $\neq 0$ only for $\varepsilon_1 < 0$. Hence, the result for the Green function can be written in a very compact form:

$$G(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \frac{A(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon - \varepsilon_1 + \mathrm{i}0\mathrm{sign}(\varepsilon)} \equiv \int_0^\infty \mathrm{d}\varepsilon_1 \frac{A^{(+)}(\varepsilon_1;\mathbf{r},\mathbf{r}')}{\varepsilon - \varepsilon_1 + \mathrm{i}0} + \int_{-\infty}^0 \mathrm{d}\varepsilon_1 \frac{A^{(-)}(\varepsilon_1;\mathbf{r},\mathbf{r}')}{\varepsilon - \varepsilon_1 - \mathrm{i}0}\,. \tag{3.79}$$

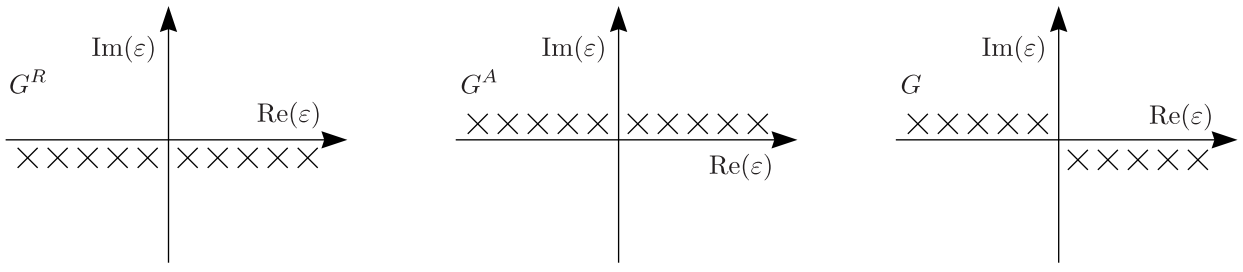
The corresponding formulae for retarded and advanced Green functions are given by:

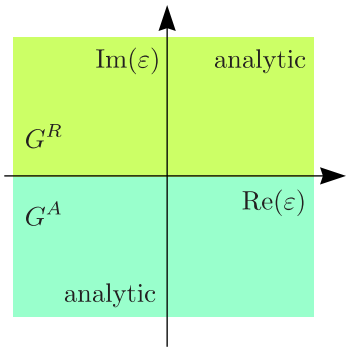
$$G^R(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \frac{A(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon - \varepsilon_1 + \mathrm{i}0}\,, \tag{3.80}$$

$$G^A(\mathbf{r},\mathbf{r}';\varepsilon) = \int \mathrm{d}\varepsilon_1 \frac{A(\mathbf{r},\mathbf{r}';\varepsilon_1)}{\varepsilon - \varepsilon_1 - \mathrm{i}0}\,. \tag{3.81}$$

Hence, we obtain:

$$G(\varepsilon) = \begin{cases} G^R(\varepsilon) & \text{for} \quad \varepsilon > 0 \\ G^A(\varepsilon) & \text{for} \quad \varepsilon < 0 \end{cases} \tag{3.82}$$





Let us assume that we have a translation invariant system in coordinate space. Then it is useful to got to momentum space:

$$G(\mathbf{r},\mathbf{r}';\varepsilon) = G(\mathbf{r}-\mathbf{r}';\varepsilon) \mapsto G(\mathbf{p};\varepsilon)\,. \tag{3.83}$$

We write $|\phi_m^{(N)}\rangle$ as $|m,N,\mathbf{p}\rangle$.

$$\widehat{\psi}(\mathbf{r}) = \sum_{\mathbf{p}} \frac{1}{\sqrt{V}} \widehat{a}_{\mathbf{p}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})\,, \tag{3.84}$$

$$G(\mathbf{p};\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{A(\mathbf{p};\varepsilon_1)}{\varepsilon - \varepsilon_1 + \mathrm{i}0\mathrm{sign}(\varepsilon)}\,. \tag{3.85}$$

$$A(\mathbf{p};\varepsilon_1) = \sum_m \Big\{ |\langle 0,N,\mathbf{p}=\mathbf{0}|\widehat{a}_{\mathbf{p}}|m,N+1,\mathbf{p}\rangle|^2 \, \delta(\varepsilon_1 - \varepsilon^{(+)}(m,\mathbf{p}),\mu) \tag{3.86}$$

$$+ |\langle m,N-1,-\mathbf{p}|\widehat{a}_{\mathbf{p}}|0,N,\mathbf{p}=\mathbf{0}\rangle|^2 \, \delta(\varepsilon_1 - \varepsilon^{(-)}(m,-\mathbf{p}) + \mu) \Big\}\,. \tag{3.87}$$

It holds that $A \in \mathbb{R}$. Hence, one obtains:

$$G^{R/A}(\mathbf{p};\varepsilon) = \int \mathrm{d}\varepsilon_1 \, \frac{A(\mathbf{p};\varepsilon_1)}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0} \Rightarrow [G^R(\mathbf{p};\varepsilon)]^* = G^A(\mathbf{p};\varepsilon)\,. \tag{3.88}$$

$$G(\mathbf{p};\varepsilon) = \begin{cases} G^R(\mathbf{p};\varepsilon) & \text{for} \quad \varepsilon > 0 \\ G^A(\mathbf{p};\varepsilon) & \text{for} \quad \varepsilon < 0 \end{cases} \tag{3.89}$$

With

$$\frac{1}{\varepsilon - \varepsilon_1 \pm \mathrm{i}0} = \mathcal{P}\frac{1}{\varepsilon - \varepsilon_1} \mp \mathrm{i}\pi\delta(\varepsilon - \varepsilon_1)\,, \tag{3.90}$$

one sees that the real parts of all Green functions is the same:

$$\mathrm{Re}(G(\mathbf{p};\varepsilon)) = \mathrm{Re}(G^R(\mathbf{p};\varepsilon)) = \mathrm{Re}(G^A(\mathbf{p};\varepsilon)) = \mathcal{P}\int \mathrm{d}\varepsilon_1 \, \frac{A(\varepsilon_1;\mathbf{p})}{\varepsilon - \varepsilon_1}\,. \tag{3.91}$$

However, the imaginary part is different:

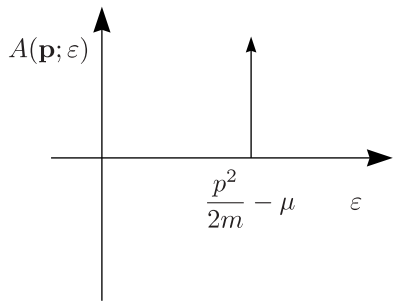
$$\left.\begin{array}{l} \mathrm{Im}(G^R(\mathbf{p};\varepsilon)) \\ \mathrm{Im}(G^A(\mathbf{p};\varepsilon)) \\ \mathrm{Im}(G(\mathbf{p};\varepsilon)) \end{array}\right\} = \pi A(\mathbf{p};\varepsilon) \begin{cases} -1 \\ +1 \\ -\mathrm{sign}(\varepsilon) \end{cases} \tag{3.92}$$

By doing some approximation these general properties should be conserved!
A nonzero spectral weight $A(\mathbf{p};\varepsilon)$ produces a pole in the Green function $G(\mathbf{p};\varepsilon)$ (excitation). In a non-interacting system it holds that

$$G(\mathbf{p};\varepsilon) = \frac{1}{\varepsilon + \mu - \frac{p^2}{2m} + \mathrm{i}0\mathrm{sign}(\varepsilon)}\,. \tag{3.93}$$

The spectral weight is given by

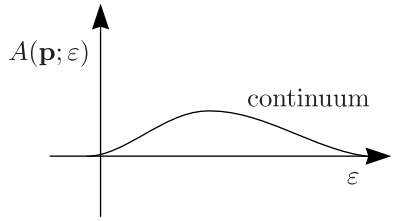
$$A(\mathbf{p};\varepsilon) = \delta\left(\varepsilon + \mu - \frac{p^2}{2m}\right)\,. \tag{3.94}$$



How does this change, when there is interaction?

$$\mathbf{p} = \sum_i \mathbf{p}_i \,. \tag{3.95}$$

One expects that $A(\mathbf{p};\varepsilon)$ will be a continuum.



Let $\mathbf{p}$ be the momentum of one quasiparticle. The Landau-Fermi-Liquid theory tells us that the pole survives. $G^{-1}(\mathbf{p};\varepsilon) = 0$ is the dispersion relation of the quasiparticles. The general structure

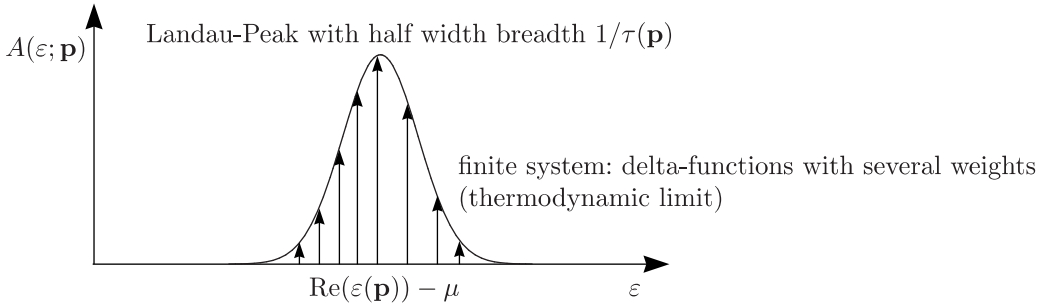
$$G(\mathbf{p};\varepsilon) = \frac{Z}{\varepsilon + \mu - \varepsilon(\mathbf{p})} \,, \tag{3.96}$$

holds with the residue Z ($0 < Z < 1$). Z is a renormalization constant (quasiparticle weight). We write the energy in the form

$$\varepsilon(\mathbf{p}) = \mathrm{Re}(\varepsilon(\mathbf{p})) + \mathrm{i}\mathrm{Im}(\varepsilon(\mathbf{p}))\,, \quad \text{with } \mathrm{Im}(\varepsilon(\mathbf{p})) = \frac{1}{2\tau(\mathbf{p})} \,, \tag{3.97}$$

where $\tau(\mathbf{p})$ is the life-time of the particle. It follows that

$$\pi A(\mathbf{p};\varepsilon) = \mathrm{Im}(G(\mathbf{p};\varepsilon)) = \frac{Z \cdot \frac{1}{2\tau(\mathbf{p})}}{\left(\varepsilon + \mu - \mathrm{Re}(\varepsilon(\mathbf{p}))\right)^2 + \left(\frac{1}{2\tau(\mathbf{p})}\right)^2} \,. \tag{3.98}$$



The imaginary part of the energy tells how quickly a state will decay.

3.7 Interaction representation

We have learned that in the Schrödinger representation states develop in time

$$\mathrm{i}\frac{\partial}{\partial t}|\phi(t)\rangle = \widehat{H}|\phi(t)\rangle \,, \quad |\phi(t)\rangle = \exp(-\mathrm{i}Ht)|\phi(0)\rangle \,, \tag{3.99}$$

and operators are time-independent. In the Heisenberg representation operators develop in time

$$\mathrm{i}\frac{\partial}{\partial t}O(t) = [O(t), \widehat{H}]\,, \quad O(t) = \exp(\mathrm{i}Ht)O(0)\exp(-\mathrm{i}Ht)\,, \tag{3.100}$$

where $O(0) \equiv O_{\mathrm{Schr}}$ and the states $|\phi\rangle$ are time-independent.
In the interaction representation we split up the Hamiltonian in the free part and the interacting part: $\widehat{H} = \widehat{H}_0 + \widehat{V}$.

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}_0\right)|\phi(t)\rangle = \widehat{V}|\phi(t)\rangle\,. \tag{3.101}$$

$\widehat{V}$ can also be t-dependent, for example by adiabatic switching: $\widehat{V} \mapsto \widehat{V}\exp(-\lambda|t|)$ with $\lambda \mapsto +0$. The states shall be time-developed by the non-interacting Hamiltonian:

$$|\phi_i(t)\rangle = \exp(\mathrm{i}H_0t)|\phi(t)\rangle\,. \tag{3.102}$$

Inserting this, we obtain:

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \widehat{H}_0\right)\exp(-\mathrm{i}H_0t)|\phi_i(t)\rangle = \widehat{V}\exp(-\mathrm{i}\widehat{H}_0t)|\phi_i(t)\rangle\,. \tag{3.103}$$

$$\mathrm{i}\frac{\partial}{\partial t}|\phi_i(t)\rangle = \widehat{V}_i(t)|\phi_i(t)\rangle\,, \quad V_i(t) = \exp(\mathrm{i}\widehat{H}_0t)\widehat{V}\exp(-\mathrm{i}\widehat{H}_0(t))\,, \quad O_i(t) = \exp(\mathrm{i}\widehat{H}_0t)\widehat{O}\exp(-\mathrm{i}\widehat{H}_0(t))\,. \tag{3.104}$$

The operators have free dynamics; they change with the free Hamiltonian H_0. But the states change as a result of the interaction. We solve the equation for $t > t_0$ with the boundary condition $|\phi_i(t)\rangle|_{t=0} = |\phi_i(t_0)\rangle$. Naively, one gets:

$$|\phi_i(t)\rangle = \exp\left(-\mathrm{i}\int\limits_{t_0}^{t}\mathrm{d}t_1\,\widehat{V}_i(t_1)\right)|\phi_i(t_0)\rangle\,. \tag{3.105}$$

However, (3.105) is **wrong**, since $[\widehat{V}_i(t'), \widehat{V}_i(t'')] \neq 0$ in general. As a result of that we solve the equation by iteration

$$|\phi_i(t)\rangle = |\phi_i(t)\rangle_0 + |\phi_i(t)\rangle_1 + |\phi_i(t)\rangle_2 + \dots\,, \tag{3.106}$$

where $|\phi_i(t)\rangle_0 \sim V^0$, $|\phi_i(t)\rangle_1 \sim V^1$, etc.

$$|\phi_i(t)\rangle_0 = |\phi_i(t_0)\rangle\,, \tag{3.107}$$

$$|\phi_i(t)\rangle_1 = (-\mathrm{i})\int\limits_{t_0}^{t}\widehat{V}_i(t_1)|\phi_i(t_1)\rangle_0\,\mathrm{d}t_1 = -\mathrm{i}\int\limits_{t_0}^{t}\widehat{V}_i(t_1)|\phi_i(t_0)\rangle\,\mathrm{d}t_1\,, \tag{3.108}$$

$$\begin{aligned}|\phi_i(t)\rangle_2 &= (-\mathrm{i})\int\limits_{t_0}^{t}\mathrm{d}t_1\,\widehat{V}_i(t_1)|\phi_i(t_1)\rangle_1 = (-\mathrm{i})^2\int\limits_{t_0}^{t}\mathrm{d}t_1\,\widehat{V}_i(t_1)\int\limits_{t_0}^{t_1}\mathrm{d}t_2\,\widehat{V}_i(t_2)|\phi_i(t_0)\rangle = \\ &= \frac{(-\mathrm{i})^2}{2}\int\limits_{t_0}^{t}\mathrm{d}t_1\int\limits_{t_0}^{t}\mathrm{d}t_2\,T[\widehat{V}_i(t_1)\widehat{V}(t_2)]|\phi_i(t_0)\rangle\,.\end{aligned} \tag{3.109}$$

The general result is given by:

$$\begin{aligned}|\phi_i(t)\rangle &= \sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\limits_{t_0}^{t}\mathrm{d}t_1\dots\int\limits_{t_0}^{t}\mathrm{d}t_n\,T[\widehat{V}_i(t_1)\dots\widehat{V}_i(t_n)]|\phi_i(t_0)\rangle \equiv \\ &\equiv T\exp\left\{-\mathrm{i}\int\limits_{t_0}^{t}\mathrm{d}t_1\,\widehat{V}_i(t_1)\right\}|\phi_i(t_0)\rangle \equiv \widehat{S}(t,t_0)|\phi_i(t_0)\rangle.\end{aligned} \tag{3.110}$$

$\widehat{S}(t,t_0)$ is the so-called evolution operator:

$$|\phi_i(t)\rangle = \widehat{S}(t,t_0)|\phi_i(t_0)\rangle\,, \tag{3.111}$$

because it contains all information, how a state in interaction representation evolves in time. Using

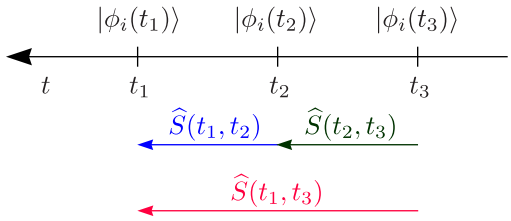
$$|\phi(t)\rangle = \exp(-\mathrm{i}\widehat{H}(t-t_0))|\phi(t_0)\rangle\,, \tag{3.112}$$

one obtains another representation for the evolution operator:

$$\widehat{S}(t,t_0) = \exp(\mathrm{i}\widehat{H}_0 t)\exp(-\mathrm{i}\widehat{H}(t-t_0))\exp(-\mathrm{i}\widehat{H}_0 t_0)\,. \tag{3.113}$$

3.7.1 Properties of the evolution operator

- $\widehat{S}(t_1,t_2)\widehat{S}(t_2,t_3) = \widehat{S}(t_1,t_3)$



- $\widehat{S}$ is unitary: $\widehat{S}^{-1}(t,t_0) = \widehat{S}^{\dagger}(t,t_0)$.
- $\widehat{S}(t_2,t_1) = \widehat{S}^{-1}(t_1,t_2) = \widehat{S}^{\dagger}(t_1,t_2)$

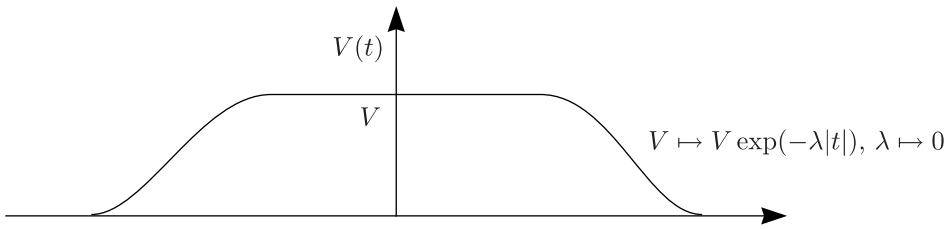
Transform the Green function into interaction representation. We assume $t_1 > t_2$.

$$G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = -\mathrm{i}\langle\phi_0|\widehat{\psi}(\mathbf{r}_1,t_1)\widehat{\psi}^{\dagger}(\mathbf{r}_2,t_2)|\phi_0\rangle\,, \tag{3.114}$$

where $|\phi_0\rangle$ is an exact many-body state. Since at $t=0$ interaction representation is the same than Schrödinger representation, we can write

$$|\phi_0\rangle = |\phi_{0,i}(0)\rangle = \widehat{S}(0,-\infty)|\phi_{0,i}(-\infty)\rangle\,. \tag{3.115}$$

We assume that at large positive and negative times the interaction is switched off.



We consider an adiabatic swtiching on/off of the interaction. So, at $t=-\infty$ we have a non-interacting ground state:

$$\phi_{0,i}(-\infty)\rangle = |0\rangle\,. \tag{3.116}$$

Now, let us look at the operators:

$$\begin{aligned}\widehat{\psi}_H(\mathbf{r},t) &= \exp(\mathrm{i}\widehat{H}t)\widehat{\psi}_S(\mathbf{r})\exp(-\mathrm{i}\widehat{H}t) = \exp(\mathrm{i}\widehat{H}t)\exp(-\mathrm{i}\widehat{H}_0 t)\widehat{\psi}_i(\mathbf{r},t)\exp(\mathrm{i}\widehat{H}_0 t)\exp(-\mathrm{i}\widehat{H}t) = \\ &= \widehat{S}^{-1}(t,0)\widehat{\psi}_i(\mathbf{r},t)\widehat{S}(t,0)\,.\end{aligned} \tag{3.117}$$

Hence, we can write the Green function as follows:

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle 0|\widehat{S}^{-1}(0,-\infty)\widehat{S}^{-1}(t_1,0)\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{S}(t_1,0)\widehat{S}^{-1}(t_2,0)\widehat{\psi}_i^{\dagger}(\mathbf{r}_2,t_2)\widehat{S}(t_2,0)\widehat{S}(0,-\infty)|0\rangle\,. \tag{3.118}$$

Using

$$\widehat{S}^{-1}(0,-\infty)\widehat{S}^{-1}(t_1,0) = \widehat{S}(-\infty,0)\widehat{S}(0,t_1) = \widehat{S}(-\infty,t_1) = \widehat{S}^{-1}(+\infty,-\infty)\widehat{S}(+\infty,t_1)\,, \tag{3.119}$$

$$\widehat{S}(t_1,0)\widehat{S}^{-1}(t_2,0) = \widehat{S}(t_1,t_2)\,, \tag{3.120}$$

and

$$\widehat{S}(t_2,0)\widehat{S}(0,-\infty) = \widehat{S}(t_2,-\infty)\,, \tag{3.121}$$

results in:

$$\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle 0|\widehat{S}^{-1}(+\infty,-\infty)\widehat{S}(+\infty,t_1)\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{S}(t_1,t_2)\widehat{\psi}_i(\mathbf{r}_2,t_2)\widehat{S}(t_2,-\infty)|0\rangle\,. \tag{3.122}$$

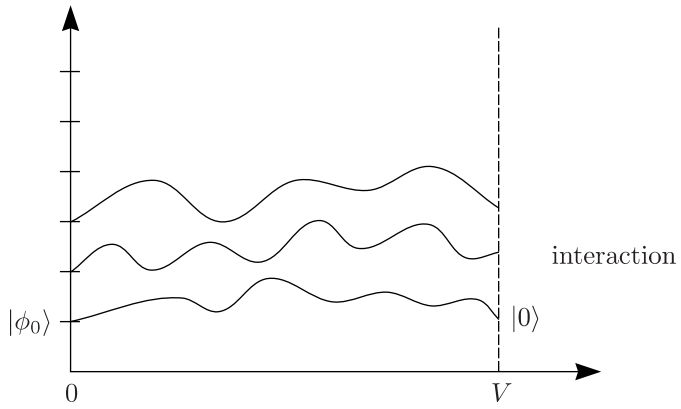
With

$$\widehat{S}(+\infty,-\infty)|0\rangle = \exp(\mathrm{i}\alpha)|0\rangle =: \langle 0|\widehat{S}|0\rangle\cdot|0\rangle\,, \tag{3.123}$$

and

$$\langle 0|S^{-1}(+\infty,-\infty) = \exp(-\mathrm{i}\alpha)\langle 0| = \langle 0|\widehat{S}|0\rangle^{-1}\cdot\langle 0|\,, \tag{3.124}$$

$$\begin{aligned}
\mathrm{i}G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) &= \frac{\langle 0|\widehat{S}(+\infty,t_1)\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{S}(t_1,t_2)\widehat{\psi}^\dagger(\mathbf{r}_2,t_2)\widehat{S}(t_2,-\infty)|0\rangle}{\langle 0|\widehat{S}|0\rangle} = \\
&= \frac{\langle 0|T[\widehat{S}\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{\psi}_i^\dagger(\mathbf{r}_2,t_2)]|0\rangle}{\langle 0|\widehat{S}|0\rangle} = \\
&= \langle 0|\widehat{S}|0\rangle^{-1}\left\langle 0\left|T\left\{\exp\left(-\mathrm{i}\int\limits_{-\infty}^{+\infty}\widehat{V}_i(t_1')\,\mathrm{d}t_1'\right)\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{\psi}_i^\dagger(\mathbf{r}_2,t_2)\right\}\right|0\right\rangle = \\
&= \langle 0|\widehat{S}|0\rangle^{-1}\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int \mathrm{d}t_1'\ldots\mathrm{d}t_n'\,\langle 0|T[\widehat{V}_i(t_1')\ldots\widehat{V}_i(t_n')\widehat{\psi}_i(\mathbf{r}_1,t_1)\widehat{\psi}_i^\dagger(\mathbf{r}_2,t)]|0\rangle\,.
\end{aligned} \tag{3.125}$$



We assume **no** spontaneous symmetry breaking.

3.8 Diagram techniques

We will change the notation: $\psi_i(\mathbf{r},t) \mapsto \psi_0(\mathbf{r},t)$. We will develop the technique for the following problem:

$$\langle 0|T[\widehat{V}_0(t_1')\ldots\widehat{V}_0(t_n')\widehat{\psi}_0(\mathbf{r}_1,t_1)\widehat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle\,, \tag{3.126}$$

with

$$\widehat{V}_0(t) = \frac{1}{2}\int \mathrm{d}r\,\mathrm{d}r'\,\widehat{\psi}_0^\dagger(\mathbf{r},t)\psi_0^\dagger(\mathbf{r}',t)\widehat{V}(\mathbf{r}-\mathbf{r}')\widehat{\psi}_0(\mathbf{r}',t)\widehat{\psi}_0(\mathbf{r},t)\,. \tag{3.127}$$

3.8.1 Wick theorem

This theorem tells us:

$$\langle 0|T[\ldots]|0\rangle = \sum \text{products of pairwise averages } (\equiv \text{contractions}) \cdot (-1)^P \,. \tag{3.128}$$

For example let us consider:

$$\begin{aligned}\langle 0|T[\widehat{\psi}_0(1)\widehat{\psi}_0^\dagger(2)\widehat{\psi}_0(3)\widehat{\psi}_0^\dagger(4)]|0\rangle = \\ = \langle 0|T\widehat{\psi}_0(1)\widehat{\psi}_0^\dagger(2)|0\rangle\langle 0|T\widehat{\psi}_0(3)\widehat{\psi}_0^\dagger(4)|0\rangle + \langle 0|T\widehat{\psi}_0(1)\widehat{\psi}_0^\dagger(4)|0\rangle \underbrace{\langle 0|T\widehat{\psi}_0^\dagger(2)\widehat{\psi}_0(3)|0\rangle}_{=-\langle 0|T\widehat{\psi}_0(3)\widehat{\psi}_0^\dagger(2)|0\rangle} = \\ = \mathrm{i}G^{(0)}(1,2)\mathrm{i}G^{(0)}(3,4) - \mathrm{i}G^{(0)}(1,4)\mathrm{i}G^{(0)}(3,2)\,.\end{aligned} \tag{3.129}$$

Let us now proof the Wick theorem. We use the notation $a_{\mathbf{p}} = b_{\mathbf{p}}^\dagger$ and $a_{\mathbf{p}}^\dagger = b_{\mathbf{p}}$ and furthermore

$$\begin{aligned}\widehat{\psi}_0(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}}\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) = \left(\sum_{|\mathbf{p}|<|\mathbf{p}_F|} + \sum_{|\mathbf{p}|>|\mathbf{p}_F|}\right) a_{\mathbf{p}}\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) = \\ = \sum_{|\mathbf{p}|<|\mathbf{p}_F|} b_{\mathbf{p}}^\dagger\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) + \sum_{|\mathbf{p}|>|\mathbf{p}_F|} a_{\mathbf{p}}\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \mathrm{i}\varepsilon_{\mathbf{p}}t) = (\widehat{\psi}_0^\dagger)^{(h)}(\mathbf{r},t) + \widehat{\psi}_0^{(p)}(\mathbf{r},t)\,,\end{aligned} \tag{3.130}$$

and analogously

$$\widehat{\psi}_0^\dagger(\mathbf{r},t) = \widehat{\psi}_0^{(h)}(\mathbf{r},t) + (\widehat{\psi}_0^\dagger)^{(p)}(\mathbf{r},t)\,. \tag{3.131}$$

It holds that $a_{\mathbf{p}}|0\rangle = 0$, $b_{\mathbf{p}}|0\rangle = 0$, $\psi_0^{(p)}|0\rangle = \psi_0^{(h)}|0\rangle = 0$. We introducte the normal product

$$N(O_1O_2\ldots) = \{\text{all } a^\dagger,\, b^\dagger \text{ to the left of all } a,\, b\} \times (-1)^P\,. \tag{3.132}$$

For example, it holds that

$$N(a_{\mathbf{p}_1}b_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_3}^\dagger b_{\mathbf{p}_4}a_{\mathbf{p}_5}a_{\mathbf{p}_6}^\dagger) = -b_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_3}^\dagger a_{\mathbf{p}_6}^\dagger a_{\mathbf{p}_1}b_{\mathbf{p}_4}a_{\mathbf{p}_5}\,. \tag{3.133}$$

The normal ordering is very useful since we can use the fact that

$$\langle 0|N(O_1O_2\ldots)|0\rangle = 0\,. \tag{3.134}$$

We define the contraction by

$$\underbrace{O_1O_2} = T(O_1O_2) - N(O_1O_2)\,, \tag{3.135}$$

and therefore obtain:

$$\langle 0|\underbrace{\widehat{\psi}_0(1)\widehat{\psi}_0^\dagger(2)}|0\rangle = \mathrm{i}G^{(0)}(1,2)\,, \tag{3.136}$$

$$\langle 0|\underbrace{\widehat{\psi}_0(1)\widehat{\psi}_0}(2)|0\rangle = 0\,. \tag{3.137}$$

The Wick theorem tells us now:

$$\begin{aligned}T(O_1O_2O_3\ldots O_n) = N(O_1O_2O_3\ldots O_n) + N(\underbrace{O_1O_2}O_3\ldots O_n) + N(\underbrace{O_1O_2}\underbrace{O_3}\ldots O_n) \\ + N(\underbrace{O_1O_2O_3\ldots O_n}) + N(O_1\underbrace{O_2O_3\ldots O_n}) + N(O_1O_2\underbrace{O_3\ldots O_n}) \\ + N(\underbrace{O_1}O_2\underbrace{O_3\ldots O_n}) + +N(\underbrace{O_1O_2O_3\ldots O_n}) + N(\underbrace{O_1}\underbrace{O_2O_3}\ldots\underbrace{O_4}) + \ldots = \\ = \sum N(\text{products with all possible contractions})\,.\end{aligned} \tag{3.138}$$

- 0-th order:

$$\mathrm{i}G^{(0)}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle 0|T[\widehat{\psi}_0(\mathbf{r}_1,t_1)\widehat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle\,. \tag{3.139}$$

- 1-th order:

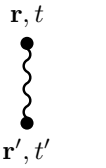
$$\langle 0|T[\widehat{V}_0(t)\widehat{\psi}_0(\mathbf{r}_1,t_1)\widehat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle = \\ = \frac{1}{2}\int \mathrm{d}r\mathrm{d}r'\, V(\mathbf{r}-\mathbf{r}')\langle 0|T[\widehat{\psi}_0^\dagger(\mathbf{r},t+0)\widehat{\psi}_0^\dagger(\mathbf{r}',t+0)\widehat{\psi}_0(\mathbf{r}',t)\widehat{\psi}_0(\mathbf{r},t)\widehat{\psi}_0(\mathbf{r}_1,t_1)\widehat{\psi}_0^\dagger(\mathbf{r}_2,t_2)]|0\rangle\,. \tag{3.140}$$

Let us analyze the matrix element. There are four $\widehat{\psi}$, which come out out interaction, and two, which are external. To tell the T-product that it should order the $\widehat{\psi}$ depending on the same time in a proper way, one adds an additional $+0$ with the $\widehat{\psi}^\dagger$, because they always come at first. This contribution gives us the following:

$$\frac{1}{2}\int \mathrm{d}r\mathrm{d}'\, V(\mathbf{r}-\mathbf{r}')\left\{-[\mathrm{i}G^{(0)}(\mathbf{r}',\mathbf{r}',-0)][\mathrm{i}G^{(0)}(\mathbf{r}_1,\mathbf{r},t_1-t)][\mathrm{i}G^{(0)}(\mathbf{r},\mathbf{r}_2,t-t_2)] + 5 \text{ more terms}\right\}\,. \tag{3.141}$$

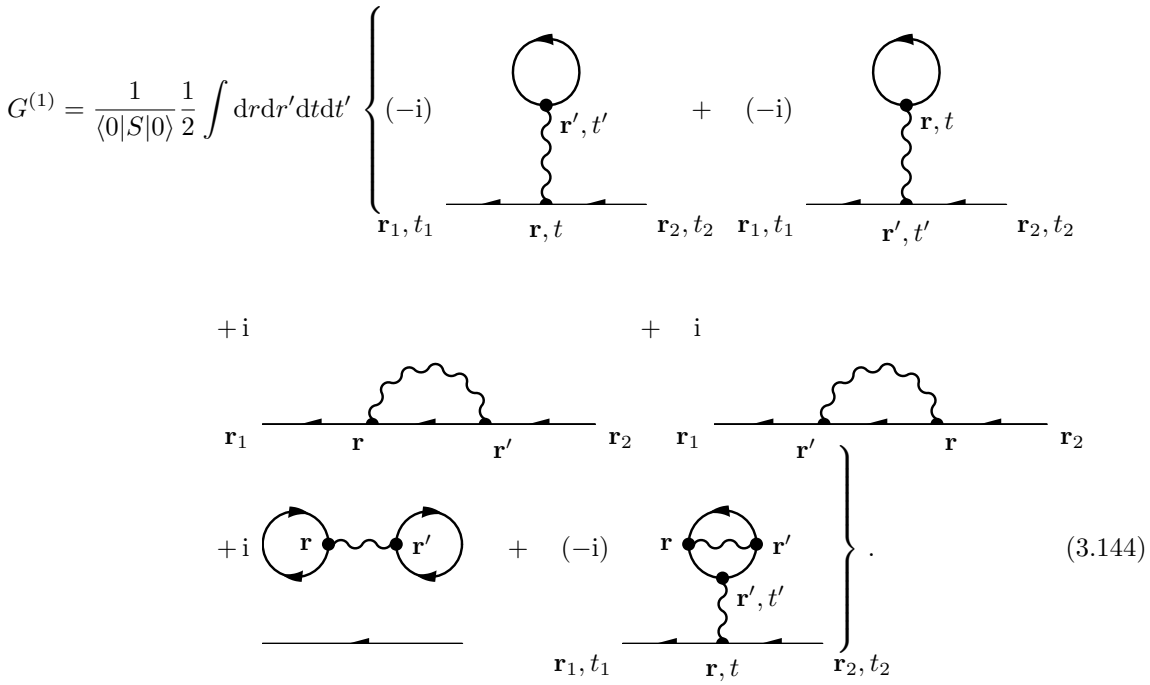
The overall sign comes from the fact that we have to put the $\widehat{\psi}^\dagger$ and $\widehat{\psi}$ in the correct order. Let us now draw diagrams for this expression. With

(3.142)



(3.143)

one obtains:

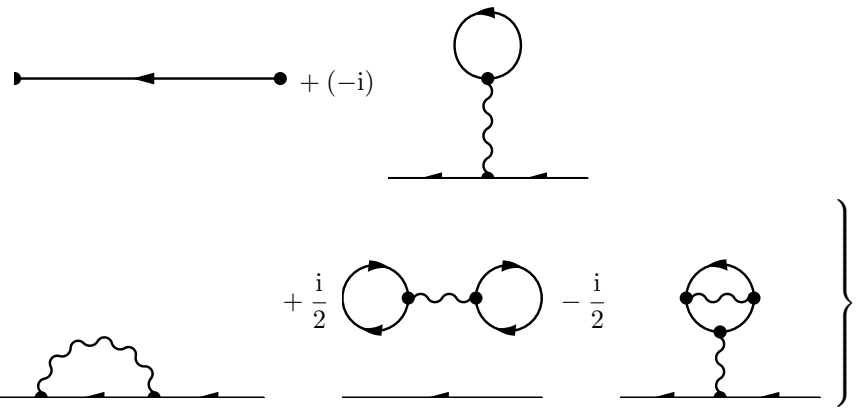


(3.144)

The number of fermionic loops produces a minus and a plus sign, respectively, depending on their number.

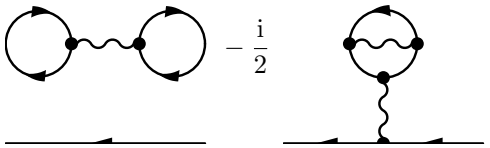
That is $(-1)^L$, where L is the number of fermionic loops. It holds that $a_1 = a_2$ and $b_1 = b_2$.

$$G = \frac{1}{\langle 0|S|0\rangle}\Bigg\{ \quad + (-\mathrm{i}) \quad + \mathrm{i} \quad + \frac{\mathrm{i}}{2} \quad - \frac{\mathrm{i}}{2} \quad \Bigg\} \tag{3.145}$$



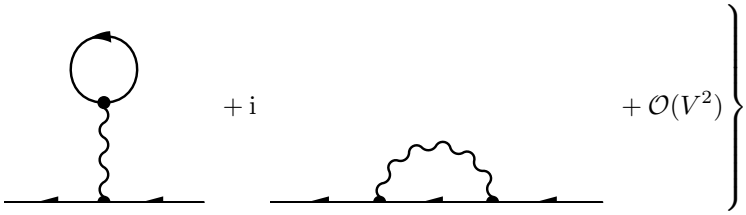
In $\langle 0|S|0\rangle$ there will be no external legs:

$$\langle 0|S|0\rangle = 1 + \frac{\mathrm{i}}{2} \quad - \frac{\mathrm{i}}{2} \quad + \dots . \tag{3.146}$$



Dividing by this eliminates the last two diagrams:

$$G = G_0 + \Bigg\{ -\mathrm{i} \quad + \mathrm{i} \quad + \mathcal{O}(V^2) \Bigg\} . \tag{3.147}$$

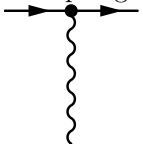


Dividing by $\langle 0|S|\rangle$ (vacuum diagrams) eliminates disconnected diagrams! This holds in general.

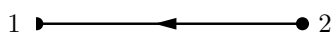
3.8.2 Rules of diagram techniques for G

Let us consider the n-th order.

1.) all topologically different diagrams with two external legs and $2n$ interaction vertices



2.) $G^{(0)}(1,2)$

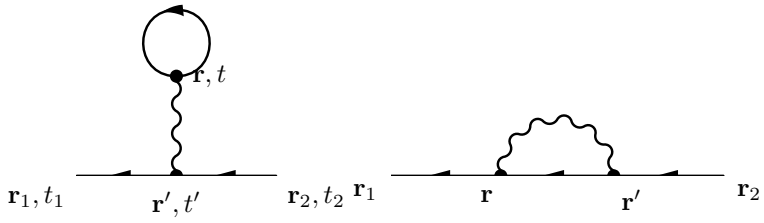


3.) $V(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$

4.) integration over t and $\mathbf{r}$ over all internal vertices, summations over spins σ (will lead to a factor $2S + 1$ for closed loops)

5.) overall factor of the diagram $\mathrm{i}^n(-1)^L$, where L is the number of closed fermionic loops

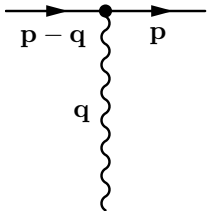
6.) $G_0(\mathbf{r}, t; \mathbf{r}', t) = G_0(\mathbf{r}, \mathbf{r}'; 0) \mapsto G_0(\mathbf{r}, \mathbf{r}', -0)$



We have the factor $1/n!$ of the time-ordered exponential and $1/2^n$ from the potential. This cancels with the number of equal diagrams. (Interchanging interaction lines gives a factor $2^n \cdot n!$.)

Because of translation invariance in space and time it is often suitable to calculate diagrams in momentum space. Hence, let us write up the diagrammatic rules in momentum space:

1.) The diagrams are the same. Each line gets some energy ε and momentum $\mathbf{p}$. There is momentum-energy conservation in each vertex.



2.)

$$G_0(\mathbf{p},\varepsilon) = \frac{1}{\varepsilon - \varepsilon_{\mathbf{p}} + \mathrm{i}0\mathrm{sign}(\varepsilon)}\,, \quad \varepsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} - \mu\,. \tag{3.148}$$

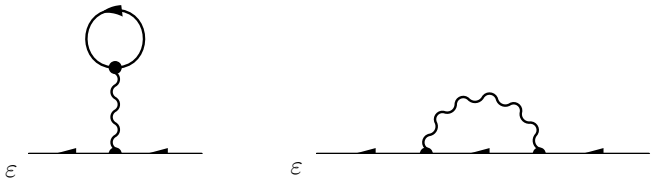
3.)

4.) integration over all n independent internal momenta and energies:

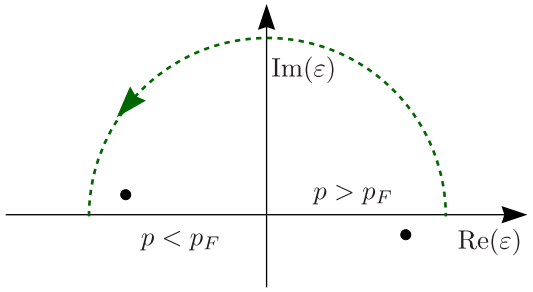
$$\int \prod_i \frac{\mathrm{d}^d p_i}{(2\pi)^d} \frac{\mathrm{d}\omega_i}{(2\pi)^d}\,. \tag{3.149}$$

5.) factor $\mathrm{i}^n(-1)^L$ (summation over spin leads to an extra factor $(2S+1)^L$)

6.) electron density



$$\int \frac{\mathrm{d}\varepsilon_1}{2\pi}\, G_0(\mathbf{p}_1,\varepsilon_1)\exp(-\mathrm{i}\varepsilon_1(-0)) = \frac{1}{2\pi} 2\pi\mathrm{i}\theta(p_F - p) = \mathrm{i}n_p\,. \tag{3.150}$$



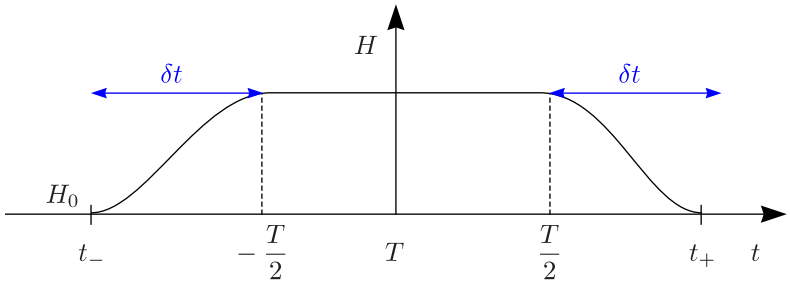
$$\int \frac{\mathrm{d}^3 p_1}{(2\pi)^3} \mathrm{i} n_p = \mathrm{i} n \,, \tag{3.151}$$

which gives the electron density.

3.9 Vacuum diagrams

They correspond to the energy of the ground state. It holds that $\langle 0|S|0\rangle = \exp(\mathrm{i}\alpha)$, where α is a phase factor. The definition of $\langle 0|S|0\rangle$ was

$$\langle 0|S|0\rangle = \langle \phi_{0,i}(-\infty)|S(+\infty,-\infty)|\phi_{0,i}(-\infty)\rangle \,. \tag{3.152}$$



It holds that $T \gg \delta T \gg$ anything else (adiabatic).

$$\langle 0|S|0\rangle = \langle \phi_{0,i}(t_-)|S(t_+,t_-)|\phi_{0,i}(t_-)\rangle \equiv \langle \phi_{0,i}(t_-)|\phi_{0,i}(t_+)\rangle \,. \tag{3.153}$$

For $t < t_-$ or $t > t_+$ the state is given by

$$|\phi_{0,i}(t)\rangle = \exp(\mathrm{i}H_0 t)|\phi_0(t)\rangle = \exp(\mathrm{i}E_0 t)|\phi_0(t)\rangle \,, \tag{3.154}$$

where $|\phi_0(t)\rangle$ is a Schrödinger state and E_0 is the ground state energy of the non-interacting system. So, we have

$$\langle 0|S|0\rangle = \exp(\mathrm{i}E_0(t_+ - t_-))\langle \phi_0(t_-)|\phi_0(t_+)\rangle \,. \tag{3.155}$$

For the time interval $t_- + \delta T < t < t_+ + \delta T$, where the interaction is switched on, the Schrödinger state $|\phi_0(t)\rangle$ is related to the Heisenberg state $|\phi_0\rangle$ by

$$|\phi_0(t)\rangle = \exp(-\mathrm{i}Et)|\phi_0\rangle \,, \tag{3.156}$$

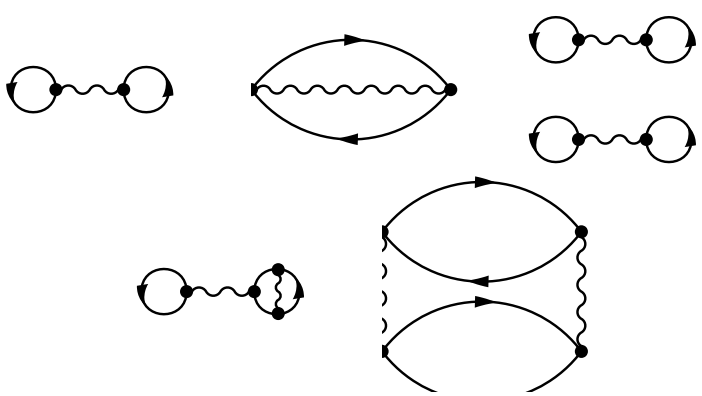
where E is the ground state energy of the interacting system. Because $T \gg \delta T$ we use this relation in the whole range T and we obtain the following result:

$$\langle 0|\widehat{S}|0\rangle = \exp(\mathrm{i}E_0(t_+ - t_-))\exp(-\mathrm{i}E(t_+ - t_-)) = \exp(-\mathrm{i}(E - E_0)T) \,. \tag{3.157}$$

We have related the change in the ground state energy $E - E_0$ due to interaction with the vacuum diagrams $\langle 0|S|0\rangle$.

$$E - E_0 = \frac{\mathrm{i}}{T} \ln(\langle 0|\widehat{S}|0\rangle \,. \tag{3.158}$$

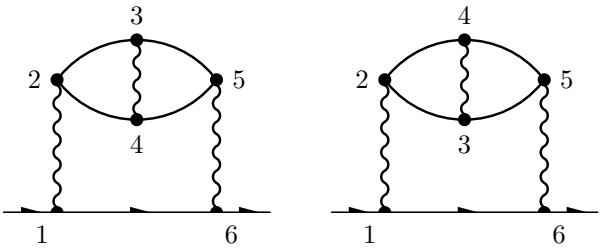
$\langle 0|\widehat{S}|0\rangle$ contains all vacuum diagrams.



There is one difference comparing to Green functions, namely the symmetry factors.

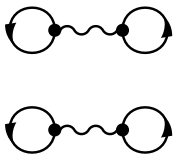
3.9.1 Symmetry factors

In Green function diagrams the factor $1/(2^n n!)$ was exactly canceled by symmetry factors, which come from interchanging the vertices (2^n) and interchanging the lines ($n!$).

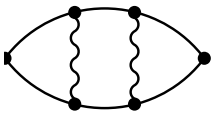


For vacuum diagrams the situation is different.

Interchanging the vertices 1 and 2 leads to the same contraction and therefore the same diagram. (It is just rotated.) The diagram has got the symmetry factor 2. The diagram



Here, the symmetry factor is 8.

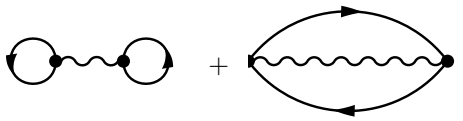


One can interchange the two lines and simultaneously 1 with 2 and 3 with 4. Hence, the overall symmetry factor is 4.
So, every diagram gets a factor $1/p$, where p represents the symmetry of the diagram.

3.9.2 Linked cluster expansion

$$E - E_0 = \frac{\mathrm{i}}{T} \ln(\langle 0|\widehat{S}|0\rangle)\Big|_{T\mapsto\infty} . \tag{3.159}$$

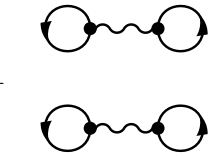
$$\langle 0|\widehat{S}|0\rangle = \sum \text{vacuum diagrams} = \underbrace{1}_{=0\text{-th}} +$$



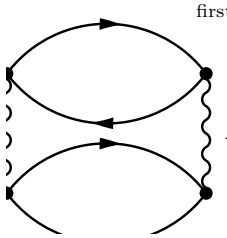
$$+$$

first order diagrams

$$+$$



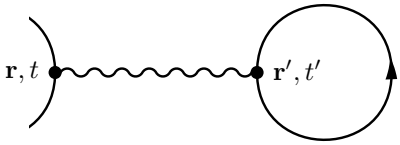
$$+$$



$$+ \ldots . \tag{3.160}$$

second order diagrams

How does the diagram



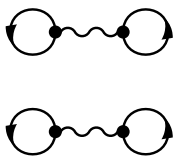
behave?

$$\int \mathrm{d}r\, \mathrm{d}r'\, \mathrm{d}t\, \mathrm{d}t'\, \frac{1}{2} G_0(\mathbf{r}, \mathbf{r}, -0) \frac{1}{2} G_0(\mathbf{r}', \mathbf{r}', -0) \delta(t - t') V(\mathbf{r} - \mathbf{r}') \sim T\,, \tag{3.161}$$

because of

$$\int \mathrm{d}t\, \mathrm{d}t'\, \delta(t - t') = T\,. \tag{3.162}$$

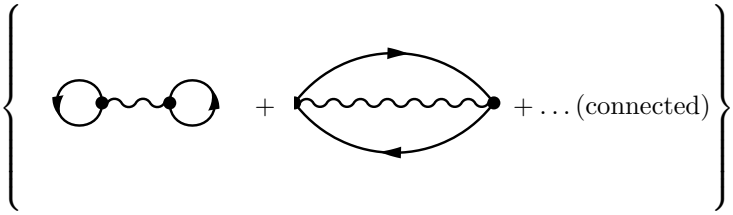
T is, for example, the life-time of the universe. So, it holds that



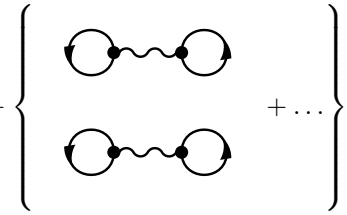
$$\sim T^2\,. \tag{3.163}$$

$$\langle 0|\widehat{S}|0\rangle = \exp(-\mathrm{i}(E - E_0)T) = 1 - \mathrm{i}(E - E_0)T + \frac{1}{2}(-\mathrm{i})^2 (E - E_0)^2 T^2 + \ldots =$$

$$= 1 +$$



$$+$$



$$+ \ldots + \ldots . \tag{3.164}$$

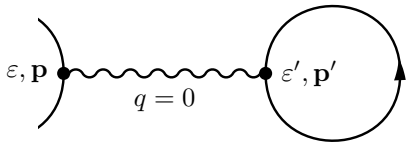
Hence, the sum of all connected diagrams is equal to $-\mathrm{i}(E-E_0)T$ („linked clusters“). From translation invariance in space it follows that any connected diagram will be proportional to the volume V. Translation invariance in space means that the underlying system is infinite.

$$\frac{E-E_0}{V} = \frac{\mathrm{i}}{T\cdot V}\Bigg\{ \quad + \quad + \quad + \quad \cdots \Bigg\}\,.$$

Hartree, 1st E_H | Fock=exchange, 1st E_{ex} | correlation energy, 2nd

(3.165)

Let us analyze the first two diagrams using the diagrammatic rules. For the Hartree diagram



we obtain:

$$\frac{E_H}{V} = \mathrm{i}^2\cdot(-1)^2\cdot\frac{1}{2}\int\frac{\mathrm{d}^d p}{(2\pi)^d}\int\frac{\mathrm{d}^d p'}{(2\pi)^d}\,\mathrm{i}n_p\cdot\mathrm{i}n_{p'}\cdot V(q=0)\cdot 2^2\,. \tag{3.166}$$

The factor $(-1)^2$ comes from the two loops and the factor 2^2 from the fermionic spin. $1/2$ is the symmetry factor of the diagram and n_p the fermionic distribution function. With

$$n_p = \begin{cases} 1 & \text{for} \quad p < p_F \\ 0 & \text{for} \quad p > p_F \end{cases}\,, \tag{3.167}$$

one obtains:

$$2\int\frac{\mathrm{d}^d p}{(2\pi)^d}\,n_p = n\,, \tag{3.168}$$

where n is the total density. The end result is then:

$$\frac{E_H}{V} = \frac{1}{2}n^2 V(q=0)\,. \tag{3.169}$$

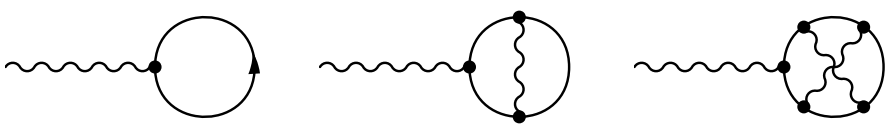
For Coulomb interaction

$$V(\mathbf{r}-\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\,, \tag{3.170}$$

the Fourier transform in three dimensions is given by

$$V(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\,. \tag{3.171}$$

At $q=0$ the potential has a singularity. This has a physical reason. For a Coulomb interaction one will have an interaction with the background, which cancels the singularity. The exact density is given by the diagrams



Let us now look at the exchange diagram:

$$\frac{E_{\text{ex}}}{V} = -\frac{1}{2}\cdot 2\int\frac{\mathrm{d}^d p}{(2\pi)^d}\int\frac{\mathrm{d}^d p'}{(2\pi)^d}\, n_p n_{p'} V(p-p')\,, \tag{3.172}$$

where $1/2$ is the symmetry factor and 2 comes from the spin. For Coulomb interaction in three dimensions the result of the integral is:

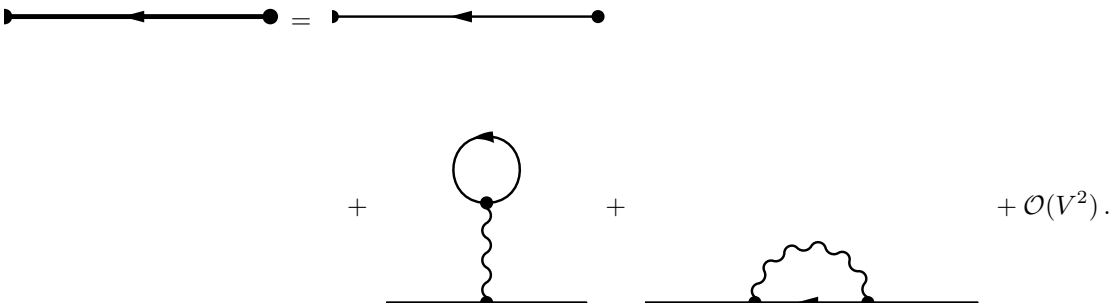
$$\frac{E_{\text{ex}}}{V} = -\frac{e^2(3\pi^2 n)^{\frac{4}{3}}}{4\pi^3}\,. \tag{3.173}$$

The sum of the two contributions is given by:

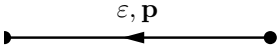
$$\boxed{\frac{E_H + E_{\text{ex}}}{V} = \int\frac{\mathrm{d}^d p}{(2\pi)^d}\int\frac{\mathrm{d}^d p'}{(2\pi)^d}\, n_p n_{p'}\left[2V(0) - V(\mathbf{p}-\mathbf{p}')\right]\,.} \tag{3.174}$$

3.10 Self-energy

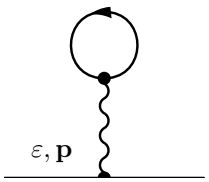
Let us go back to the expansion of Green functions:



(3.175)

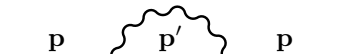


$$= \frac{1}{\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon)} \equiv G^{(0)}(\mathbf{p},\varepsilon)\,, \quad \varepsilon_p = \frac{p^2}{2m} - \mu\,. \tag{3.176}$$



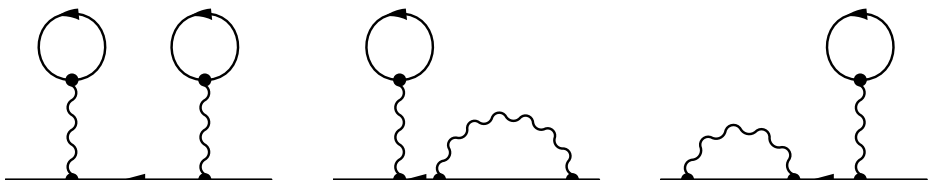
$$= \mathrm{i}\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon))^2} V(0)\mathrm{i}\int\frac{\mathrm{d}^3 p'}{(2\pi)^3}\, n_{p'}(-1) = \frac{nV(0)}{(\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon))^2}\,. \tag{3.177}$$

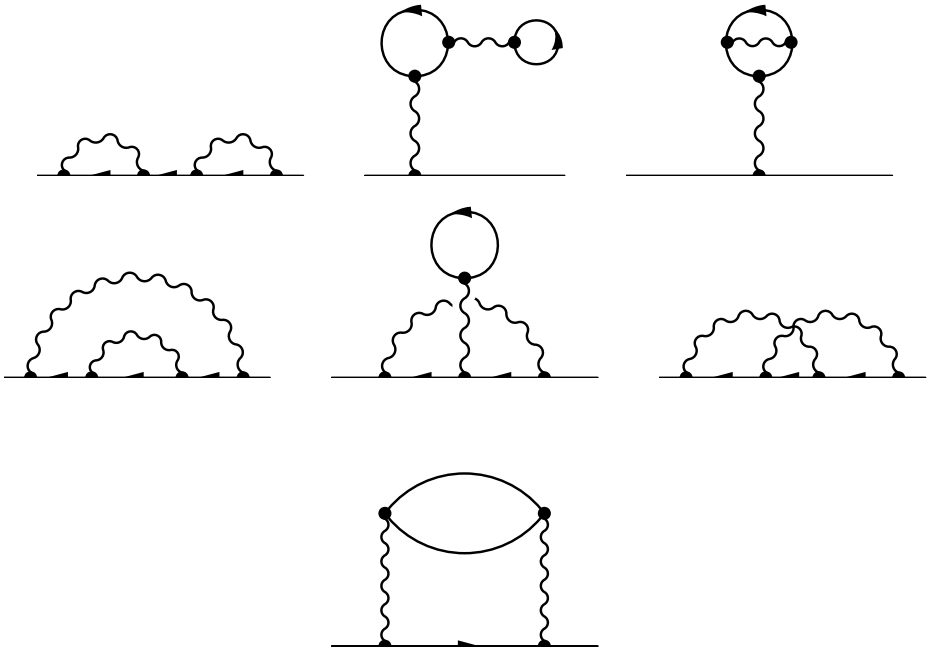
In presence of spin we have to multiply with an additional factor 2.



$$= -\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon))^2}\int\frac{\mathrm{d}^d p'}{(2\pi)^3}\, V(\mathbf{p}-\mathbf{p}')n_{p'}\,. \tag{3.178}$$

Let us go to the second order:





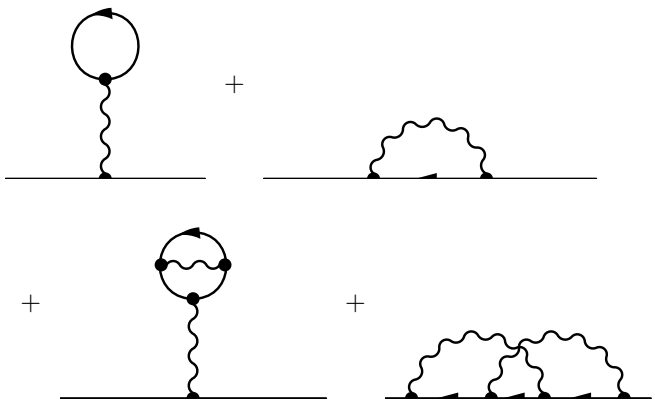
All diagrams in (I) will contain the factor

$$\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon))^3}\,, \tag{3.179}$$

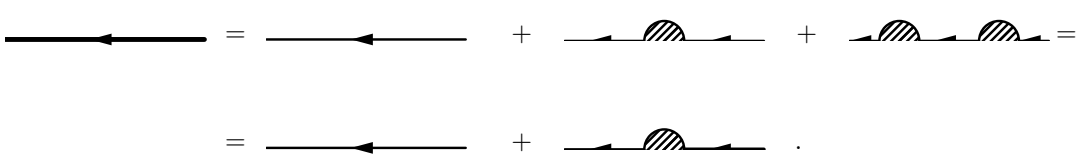
and all diagrams in (II) the factor

$$\frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon))^2}\,. \tag{3.180}$$

Self-energy:

$\Sigma(\mathbf{p},\varepsilon) =$  (3.181)

which is the sum of all diagrams that cannot be separated in two parts by cutting the electronic line. We can now write the Green function in the following form:

 (3.182)

$$G = G^{(0)} + G^{(0)}\Sigma G\,, \tag{3.183}$$

or

$$G^{-1} = (G^{(0)})^{-1} - \Sigma\,. \tag{3.184}$$

$$G(\varepsilon,\mathbf{p}) = \frac{1}{(G^{(0)})^{-1}(\varepsilon,\mathbf{p}) - \Sigma(\varepsilon,\mathbf{p})} = \frac{1}{\varepsilon - \varepsilon_p + \mathrm{i}0\mathrm{sign}(\varepsilon) - \Sigma(\varepsilon,\mathbf{p})}\,. \tag{3.185}$$

From the Lehmann expansion it followed that

$$\mathrm{sign}(\mathrm{Im}(G(\varepsilon,\mathbf{p}))) = -\mathrm{sign}(\varepsilon)\,, \tag{3.186}$$

which means

$$\mathrm{sign}(\mathrm{Im}(\Sigma(\varepsilon,\mathbf{p}))) = -\mathrm{sign}(\varepsilon)\,. \tag{3.187}$$

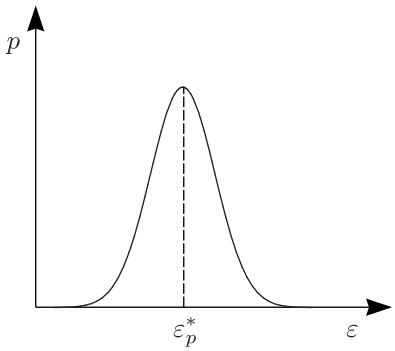
Σ will by itself produce the proper sign.

It can be divided into its real and imaginary part:

$$\Sigma(\mathbf{p},\varepsilon) = \mathrm{Re}(\Sigma(\mathbf{p},\varepsilon)) + \mathrm{i}\mathrm{Im}(\Sigma(\mathbf{p},\varepsilon))\,. \tag{3.188}$$

The spectral weight is given by

$$A(\mathbf{p},\varepsilon) = -\frac{1}{\pi}\mathrm{Im}(G(\mathbf{p},\varepsilon))\mathrm{sign}(\varepsilon) = \frac{|\mathrm{Im}(\Sigma(\mathbf{p},\varepsilon))|}{|\varepsilon - \varepsilon_p - \mathrm{Re}(\Sigma(\mathbf{p},\varepsilon))|^2 + |\mathrm{Im}(\Sigma(\mathbf{p},\varepsilon))|^2}\,. \tag{3.189}$$



quasiparticle dispersion

ε_p^* is the solution of the equation

$$\varepsilon - \varepsilon_p - \mathrm{Re}(\Sigma(\mathbf{p},\varepsilon)) = 0\,. \tag{3.190}$$

Hence, we can write

$$\varepsilon_p^* = \varepsilon_p + \mathrm{Re}(\Sigma(\mathbf{p},\varepsilon^*))\,. \tag{3.191}$$

We make an expansion with respect to ε_p^*:

$$\varepsilon - \varepsilon_p - \mathrm{Re}(\Sigma(\mathbf{p},\varepsilon)) \simeq \underbrace{\left[1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}(\Sigma(\mathbf{p},\varepsilon))\Big|_{\varepsilon_p=\varepsilon_p^*}\right]}_{Z_p^{-1}}(\varepsilon - \varepsilon_p^*)\,. \tag{3.192}$$

For the Green function it then results that

$$G(\varepsilon,\mathbf{p}) \simeq \frac{1}{Z_p^{-1}(\varepsilon - \varepsilon_p^*) - \mathrm{i}\mathrm{Im}(\Sigma(\varepsilon,\mathbf{p}))} = \frac{Z_p}{\varepsilon - \varepsilon_p^* - \frac{\mathrm{i}}{2}\Gamma(\varepsilon,\mathbf{p})}\,, \quad \Gamma(\varepsilon,\mathbf{p}) = Z_p\mathrm{Im}(\Sigma(\varepsilon,\mathbf{p}))\,. \tag{3.193}$$

We realize that

- the quasiparticle dispersion relation changes: $\varepsilon_p \mapsto \varepsilon_p^*$. The quasiparticle obtains an effective mass.
- The residue is no longer equal to one. It holds that $0 < Z_p < 1$, so it remains a Fermi liquid.
- $\Gamma(\varepsilon_p^*,\mathbf{p})$ is the decay rate of the quasiparticle.

The dispersion of non-interacting particles is linear near the Fermi surface:

$$\varepsilon_p \simeq v_F(\mathbf{p}-\mathbf{p}_F)\,, \quad \frac{p_F}{v_F} = m\,. \tag{3.194}$$

We linearize

$$\varepsilon - \varepsilon_p - \mathrm{Re}(\Sigma(\varepsilon,\mathbf{p}))\,, \tag{3.195}$$

and obtain:

$$\left[1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}(\Sigma(\mathbf{p},\varepsilon))\Big|_{\substack{\varepsilon=0\\ \mathbf{p}=\mathbf{p}_F}}\right]\varepsilon - v_F(\mathbf{p}-\mathbf{p}_F)\left[1 + \frac{\partial}{\partial\varepsilon_p}\mathrm{Re}(\Sigma(\varepsilon,\mathbf{p}))\Big|_{\substack{\varepsilon=0\\ \mathbf{p}=\mathbf{p}_F}}\right] = 0\,. \tag{3.196}$$

We define

$$\varepsilon = (\mathbf{p}-\mathbf{p}_F)v_F^* \equiv \varepsilon_p^*\,, \tag{3.197}$$

and obtain for the effective mass:

$$m^* = \frac{p_F}{v_F^*} = m\frac{1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}(\Sigma(\mathbf{p},\varepsilon))\Big|_{\substack{\varepsilon=0\\ \mathbf{p}=\mathbf{p}_F}}}{1 + \frac{\partial}{\partial\varepsilon_p}\mathrm{Re}(\Sigma(\varepsilon,\mathbf{p}))\Big|_{\substack{\varepsilon=0\\ \mathbf{p}=\mathbf{p}_F}}}\,, \tag{3.198}$$

or

$$\frac{m}{m^*} = Z\left[1 + \frac{\partial}{\partial\varepsilon_p}\mathrm{Re}(\Sigma(\mathbf{p},\varepsilon))\Big|_{\substack{\mathbf{p}=\mathbf{p}_F\\ \varepsilon=0}}\right]\,, \quad Z = Z_{\mathbf{p}=\mathbf{p}_F}\,. \tag{3.199}$$

We want to look at the distribution of particles in a Fermi-liquid with respect to momenta.

$$G(\mathbf{p},\varepsilon) \simeq \frac{Z}{\varepsilon - v_F^*(\mathbf{p}-\mathbf{p}_F) + \mathrm{i}0\mathrm{sign}(\varepsilon)} + G_{\mathrm{incoh}}(\mathbf{p},\varepsilon)\,, \tag{3.200}$$

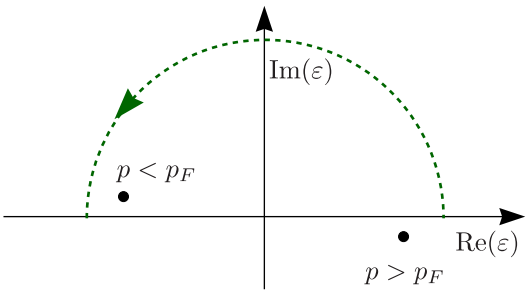
where we have replaced $\Gamma/2$ by zero because of $\Gamma \mapsto 0$ for $\varepsilon \mapsto 0$ and $\mathbf{p} \mapsto \mathbf{p}_F$. The density is given by

$$\varrho(\mathbf{r}) = \langle 0|\psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t)|0\rangle = -\mathrm{i}G(\mathbf{r},\mathbf{r};t=-0) = -\mathrm{i}\int\frac{\mathrm{d}^dp}{(2\pi)^d}\,G(\mathbf{p},t=-0)\,. \tag{3.201}$$

For calculating

$$n_p = -\mathrm{i}G(\mathbf{p},t=-0) = -\mathrm{i}\lim_{t\mapsto-0}\int\frac{\mathrm{d}\varepsilon}{2\pi}\,G(\mathbf{p},\varepsilon)\exp(-\mathrm{i}\varepsilon t)\,, \tag{3.202}$$

we have to look, where the poles are.



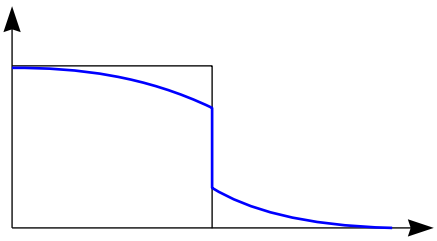
Because of

$$\frac{Z}{\varepsilon - \mathbf{v}_F^*(\mathbf{p}-\mathbf{p}_F) + \mathrm{i}0\mathrm{sign}(p_F)}\,, \tag{3.203}$$

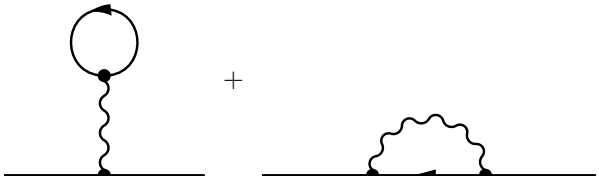
for $p < p_F$ the contribution will be Z and for $p > p_F$ it will be zero.

$$n_{p_F-0} - n_{p_F+0} = Z\,. \tag{3.204}$$

From this picture we understand that it should hold that $0 < Z < 1$.



For $Z = 1$ we have a non-interacting system and for $Z > 0$ a Fermi liquid. In the first order we have to look at the diagrams Hartree and Fock (exchange):

$\Sigma^{(1)}(\mathbf{p}, \varepsilon) =$  $=$

$$= \int \frac{\mathrm{d}^3 p'}{(2\pi)^3} \, n_{p'}^{(0)} [2V(0) - V(\mathbf{p} - \mathbf{p}')] \,, \quad n_p^{(0)}(\mu) = \theta(\mathbf{p}_F^{(0)}(\mu) - \mathbf{p}) \,. \tag{3.205}$$

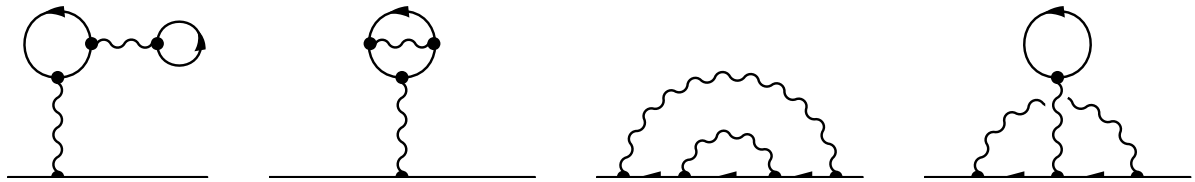
The factor 2 in the first summand comes from spin. What are the properties of $\Sigma^{(1)}(\mathbf{p}, \varepsilon)$?

- It is real: $\mathrm{Im}(\Sigma^{(1)}(\mathbf{p}, \varepsilon)) = 0$.
- It is independent of the energy ε.
- It holds that $\tau = \Gamma^{-1} = \infty$, where τ is the life time and Γ the decay rate. Hence, the quasi-particle will not decay.
- We don't get any renormalization; it still holds that $Z = 1$, because $\Sigma^{(1)}(\mathbf{p}, \varepsilon)$ does not depend on the energy.
- Since Σ_{exchange} is dependent on the momentum $\mathbf{p}$ we obtain $m^* \neq m$; hence the mass will be renormalized.

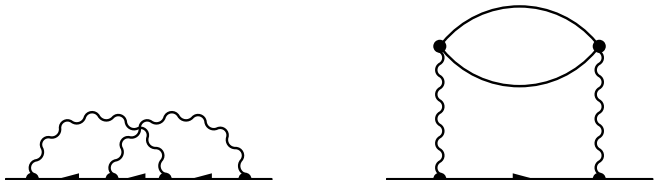
Let us now look at second order corrections:

$$\Sigma^{(2)} = \Sigma^{(2a)} + \Sigma^{(2b)} \,, \tag{3.206}$$

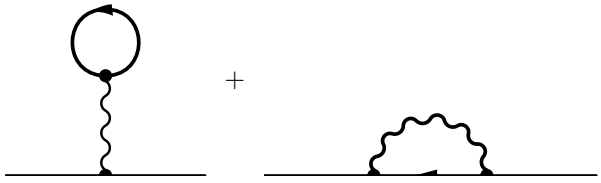
where the diagrams (2a) are given by



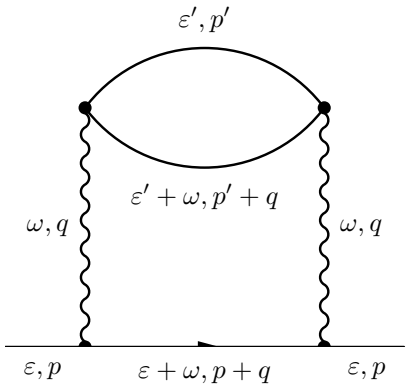
and the diagrams (2b) by



Then, we can write

$\Sigma^{\mathrm{HF}} =$  $,$ (3.207)

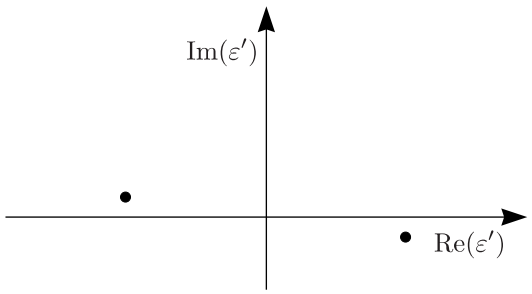
which is called self-consistent Hartree-Fock. In its calculation one only has to replace $n_p^{(0)}(\mu)$ by $n_p(\mu)$ in the bare Hartree-Fock expression. If one wants to compute the effective mass, they are, of course, important, but not for the examination of the life-time. Hence, we have to look at the diagrams (2b).



$$-\mathrm{i}^2 \int \frac{\mathrm{d}\omega\, \mathrm{d}^3q\, \mathrm{d}\varepsilon'\, \mathrm{d}^3p'}{(2\pi)^8}\, V^2(\mathbf{q}) \frac{1}{\varepsilon + \omega - \varepsilon_{p+q} + \mathrm{i0sign}(|\mathbf{p}+\mathbf{q}| - p_F)} \times$$
$$\times \frac{1}{\varepsilon' + \omega - \varepsilon_{p'+q} + \mathrm{i0sign}(|\mathbf{p}'+q| - p_F)} \cdot \frac{1}{\varepsilon' - \varepsilon_{p'} + \mathrm{i0sign}(p' - p_F)} \,. \tag{3.208}$$

Let us look at the integral over ε':

$$\int \frac{\mathrm{d}\varepsilon'}{2\pi} \frac{1}{\varepsilon' + \omega - \varepsilon_{p'+q} + \mathrm{i0sign}(|\mathbf{p}'+\mathbf{q}| - p_F)} \cdot \frac{1}{\varepsilon' - \varepsilon_{p'} + \mathrm{i0sign}(p' - p_F)} =$$
$$= \frac{2\pi\mathrm{i}}{2\pi} \frac{1}{\varepsilon_{p'} - \varepsilon_{p'+q} + \omega + \mathrm{i0sign}(|\mathbf{p}'+\mathbf{q} - p_F)} \left[\theta(|\mathbf{p}'+\mathbf{q}| - p_F) - \theta(p' - p_F)\right] . \tag{3.209}$$



Now, we come to the integral over ω, which yields to the following result:

$$\mathrm{i} \frac{1}{\varepsilon - \varepsilon_{p+q} - \varepsilon_{p'} + \varepsilon_{p'+q} + \mathrm{i0sign}(|p+q| - p_F)} \left[\theta(|p+q| - p_F) - \theta(|p'+q| - p_F)\right] . \tag{3.210}$$

There are two possibilities to get a non-zero product

$$\left[\theta(|p+q| - p_F) - \theta(|p'+q| - p_F)\right] \left[\theta(|\mathbf{p}'+\mathbf{q}| - p_F) - \theta(p' - p_F)\right] , \tag{3.211}$$

namely

$$|p'+q| > p_F \,, \quad p' < p_F \,, \quad |p+q| < p_F \,, \tag{3.212}$$

or

$$|p'+q| < p_F \,, \quad p' > p_F \,, \quad |p+q| > p_F \,. \tag{3.213}$$

$$\Sigma^{(2\mathrm{b})_1}(\mathbf{p}, \varepsilon) = \int \frac{\mathrm{d}^3q\, \mathrm{d}^3p}{(2\pi)^6}\, V^2(q) \frac{1}{\varepsilon - \varepsilon_{p+q} - \varepsilon_{p'} + \varepsilon_{p'+q} + \mathrm{i0sign}(|p+q| - p_F)} \times$$
$$\times \left[(1 - n_{p'+q}) n_{p'} n_{p+q} + n_{p'+q}(1 - n_{p'})(1 - n_{p+q})\right] , \tag{3.214}$$

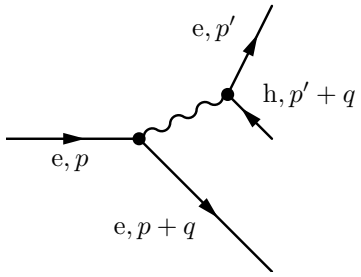
where n_p is the Fermi distribution function. We are interested in the imaginary part using

$$\mathrm{Im}\frac{1}{x+\mathrm{i}0} = -\pi\delta(x)\,, \tag{3.215}$$

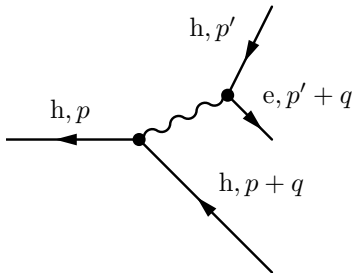
and obtain:

$$\begin{aligned}\mathrm{Im}(\Sigma^{(2\mathrm{b})_1}(\mathbf{p},\varepsilon)) = \pi \int \frac{\mathrm{d}^3p\,\mathrm{d}^3p'}{(2\pi)^6}\,\delta\left(\varepsilon - \varepsilon_{p+q} - \varepsilon_{p'} + \varepsilon_{p'+q}\right) U^2(q)\times \\ \times\left[(1-n_{p'+q})n_{p'}n_{p+q} - n_{p'+q}(1-n_{p'})(1-n_{p+q})\right]\,.\end{aligned} \tag{3.216}$$

The first term in non-zero, if it holds that $\varepsilon_{p'+q} > 0$, $\varepsilon_{p'} < 0$ and $\varepsilon_{p+q} < 0$ and therefore $\varepsilon < 0$. For the second term it holds that $\varepsilon_{p'+q} < 0$, $\varepsilon_{p'} > 0$ and $\varepsilon_{p+q} > 0$, which gives $\varepsilon > 0$. Hence, the first term gives a contribution for particles below the Fermi surface and the second term a contribution for particles above the Fermi surface.



That is the physical process e → eeh. An incoming electron will use some of its energy to excite an electron in the Fermi sea, such that an electron-hole pair appears.
The second term corresponds to h → hhe.



Chapter 4

Linear response

We look at the Hamiltonian

$$\widehat{H} \mapsto \widehat{H} + \widehat{A} f(t)\,, \tag{4.1}$$

where $f(t')$ describes the perturbation in time. We are interested in $\delta B(t) = B(t) - B_0(t)$ with $B(t) = \langle\phi(t)|\widehat{B}(t)|\phi(t)\rangle$. It holds that

$$\delta B(t) = -\mathrm{i}\int\limits_{-\infty}^{t} \mathrm{d}t'\,\langle\phi_0|[\widehat{B}(t),\widehat{A}(t')]|\phi_0\rangle f(t') \equiv \int \mathrm{d}t'\,\mathscr{D}^R_{BA}(t,t') f(t')\,, \tag{4.2}$$

with

$$\mathscr{D}^R_{BA}(t,t') = -\mathrm{i}\theta(t-t')\langle\phi_0|[\widehat{B}(t),\widehat{A}(t')]|\phi_0\rangle\,, \tag{4.3}$$

where the index R means "retarded". It will be a function of $t-t'$, if the Hamiltonian is time-independent. The linear response function $\mathcal{D}^R_{BA}(t,t')$, which describes how the observables change due to the perturbation, is called **Kubo formula**. Let us now consider as perturbation a scalar potential: $f(t) \mapsto \varphi(x,t)$. The operator, which the potential couples, is the density operator

$$\widehat{A}(t) \mapsto \widehat{\varrho}(x,t) = \psi^\dagger(x,t)\psi(x,t)\,, \tag{4.4}$$

and the perturbation of the Hamiltonian is given by

$$\delta H = \int \mathrm{d}x\,\varphi(x,t)\widehat{\varrho}(x,t)\,, \tag{4.5}$$

where we have to integrate over all spatial points x, because the perturbation acts at every point. Since we consider the perturbation coupled to density, the observable will also be a density: $B(t) = \widehat{\varrho}(x,t)$. Hence, we will obtain the density-density response function

$$\mathscr{D}^R_{\varrho\varrho}(x-x',t-t') = -\mathrm{i}\theta(t-t')\langle\phi_0|[\widehat{\varrho}(x,t),\widehat{\varrho}(x',t')]|\phi_0\rangle = \Pi^R(x-x',t-t')\,, \tag{4.6}$$

and it is called polarization operator (functional). It determined the response of the density with the change of the potential:

$$\delta\varrho(x,t) = \int \mathrm{d}x'\,\mathrm{d}t'\,\Pi^R(x-x',t-t')\varphi(x',t')\,. \tag{4.7}$$

The diagrammatic approach allows us to calculate

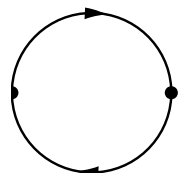
$$\mathscr{D}_{BA}(t,t') = -\mathrm{i}\langle\phi_0|T\widehat{B}(t)\widehat{A}(t')|\phi_0\rangle\,. \tag{4.8}$$

Analogously to Green functions one can write

$$\mathscr{D}_{BA}(\omega) = \begin{cases} \mathscr{D}^R_{BA}(\omega) & \text{for} \quad \omega > 0 \\ \mathscr{D}^A_{BA}(\omega) = [D^R_{BA}(\omega)]^* & \text{for} \quad \omega < 0 \end{cases}\,. \tag{4.9}$$

Therefore, we have to look at

$$\Pi(x,t) = -\mathrm{i}\langle\phi_0|T\widehat{\varrho}(x,t)\widehat{\varrho}(0,0)|\phi_0\rangle = -\mathrm{i}\Big\{$$



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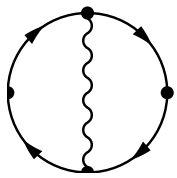

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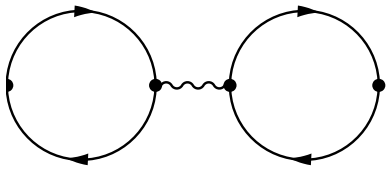
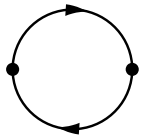


$\Big\}$ (4.10)

By using the diagrammatic rules we calculate the non-interacting part of $\Pi(q,\omega)$.

$$\Pi(q,\omega) = -\mathrm{i}$$



$$= (-\mathrm{i})(-1)\int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\mathrm{d}\varepsilon}{2\pi}\frac{1}{\varepsilon+\frac{\omega}{2}-\frac{1}{2m}\left(\mathbf{p}-\frac{\mathbf{q}}{2}\right)^2+\mu+\mathrm{i}0\mathrm{sign}\left(\varepsilon+\frac{\omega}{2}\right)}\times$$
$$\times\frac{1}{\varepsilon-\frac{\omega}{2}-\frac{1}{2m}\left(\mathbf{p}-\frac{\mathbf{q}}{2}\right)^2+\mu+\mathrm{i}0\mathrm{sign}\left(\varepsilon-\frac{\omega}{2}\right)}\,. \tag{4.11}$$

We will consider the limit $|\mathbf{q}| \ll k_F$, because it will simplify the calculation. Hence, we can write

$$\frac{1}{2m}\left(\mathbf{p}\pm\frac{\mathbf{q}}{2}\right)^2-\mu \simeq \underbrace{\frac{\mathbf{p}^2}{2m}-\mu}_{\equiv\xi}\pm\frac{\mathbf{p}\cdot\mathbf{q}}{2m} \simeq \xi \pm \frac{1}{2}v_F\mathbf{n}\cdot\mathbf{q}\,, \tag{4.12}$$

and it follows that (with the density of states ν at the Fermi surface):

$$\Pi(q,\omega) = \mathrm{i}\int \nu\,\mathrm{d}\xi\,\mathrm{d}\mathbf{n}\frac{\mathrm{d}\varepsilon}{2\pi}\frac{1}{\varepsilon-\xi+\frac{1}{2}\left(\omega-v_F\mathbf{n}\cdot\mathbf{q}\right)+\mathrm{i}0\mathrm{sign}\left(\xi+v_F\cdot\frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)}\times$$
$$\times\frac{1}{\varepsilon-\xi-\frac{1}{2}\left(\omega-v_F\mathbf{n}\cdot\mathbf{q}\right)+\mathrm{i}0\mathrm{sign}\left(\xi-v_F\frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)}\,. \tag{4.13}$$

We will first do the integral over the energy. The energy integration does not vanish, if

$$\mathrm{sign}\left(\xi+v_F\frac{\mathbf{n}\cdot\mathbf{q}}{2}\right) \neq \mathrm{sign}\left(\xi-v_F\frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)\,, \tag{4.14}$$

holds (because then, the poles lie on different sides) and therefore

$$-v_F\frac{|\mathbf{n}\cdot\mathbf{q}|}{2} < \xi < v_F\frac{|\mathbf{n}\cdot\mathbf{q}|}{2}\,. \tag{4.15}$$

We the obtain

$$\Pi(q,\omega) = \mathrm{i}\nu\frac{2\pi\mathrm{i}}{2\pi}\int\limits_{-\frac{1}{2}v_F|\mathbf{n}\cdot\mathbf{q}|}^{\frac{1}{2}v_F|\mathbf{n}\cdot\mathbf{q}|}\mathrm{d}\xi\,\mathrm{d}\mathbf{n}\,\frac{1}{\omega-v_F\mathbf{n}\cdot\mathbf{q}+\mathrm{i}0\mathrm{sign}(\mathbf{n}\cdot\mathbf{q})}\mathrm{sign}(\mathbf{n}\cdot\mathbf{q}) =$$
$$= \nu\int\mathrm{d}\mathbf{n}\,\frac{-v_F\mathbf{n}\cdot\mathbf{q}}{\omega-v_F\mathbf{n}\cdot\mathbf{q}+\mathrm{i}0\mathrm{sign}(\omega)} = \nu\left[1-\frac{s}{2}\ln\left(\frac{s+1}{s-1}\right)\right]\,, \tag{4.16}$$

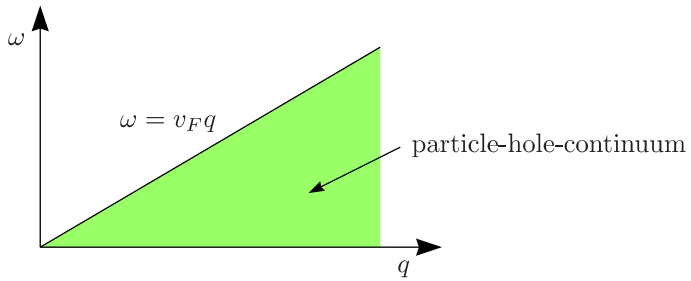
with $s = (\omega+\mathrm{i}0\mathrm{sign}(\omega))/(qv_F)$. We consider the limit

$$\lim_{q\mapsto 0}\lim_{\omega\mapsto 0}\Pi(q,\omega) = \nu\,, \tag{4.17}$$

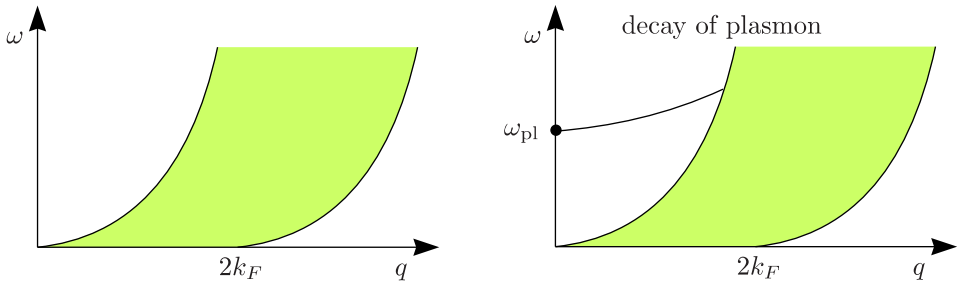
which yields a static screening (Thomas-Fermi screening).

$$\lim_{\omega \mapsto 0} \lim_{q \mapsto 0} \Pi(q, \omega) = 0\,, \tag{4.18}$$

which corresponds to $s \mapsto \infty$. The polarization operator is a response to an external potential. In this case, the system will not realize that the potential exists. If a scalar potential is uniform, it does not produce an electric field. Then it can be simply gauged (gauge invariance).
Where does $\mathrm{Im}(\Pi(q, \omega))$ not vanish? It holds for $\omega < v_F q$. So, the imaginary part corresponds to the dissipation; electron-hole pairs will be produced.



This behavior holds for $q \ll k_F$. In general, one obtains the following picture:



4.1 Coulomb interaction: screening, random phase approximation (RPA)

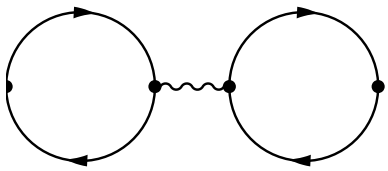
We consider

$$V(\mathbf{r}) = \frac{e^2}{|\mathbf{r}|}\,, \tag{4.19}$$

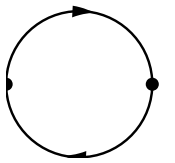
and in three dimensions it holds that

$$V(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\,. \tag{4.20}$$

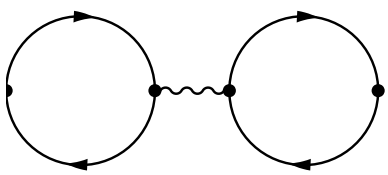
$V(\mathbf{q})$ is singular at $|\mathbf{q}| \mapsto 0$ and therefore produces divergencies. For example:



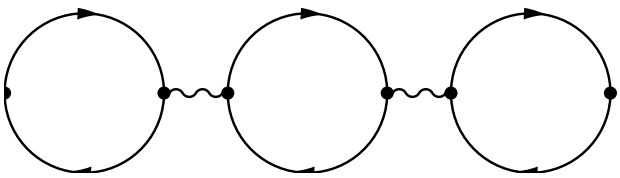
$$\sim \int \mathrm{d}^3 q \left(\frac{1}{q^2}\right)^2 = \infty\,. \tag{4.21}$$



$$:\quad \frac{1}{q^2}$$

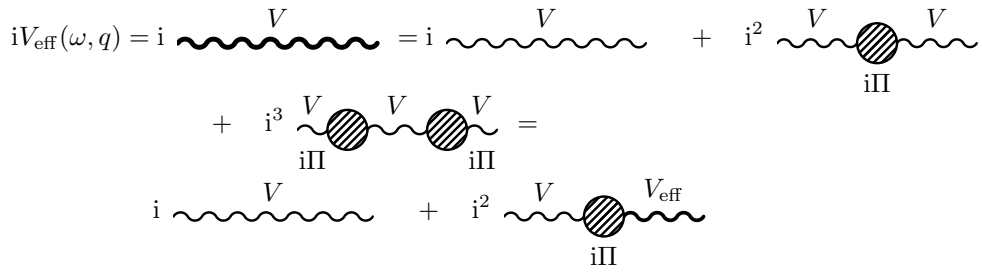


$$:\quad \frac{1}{q^4}$$



$$: \quad \frac{1}{q^6}$$

We have to sum up all contributions, which produces an effective potential V_{eff}:



(4.22)

Hence, we can write

$$\mathrm{i}V_{\text{eff}} = \mathrm{i}V + \mathrm{i}V\mathrm{i}\Pi\mathrm{i}V_{\text{eff}}\,, \tag{4.23}$$

and therefore

$$V_{\text{eff}}(\omega, q)\left[1 + V(q)\Pi(\omega, q)\right] = V(\omega, q)\,, \tag{4.24}$$

$$\boxed{V_{\text{eff}}(\omega, q) = \frac{V(q)}{1 + V(q)\Pi(\omega, q)}\,.} \tag{4.25}$$

V_{eff} is no longer singular. The technique here is called random phase approximation (RPA). The effective interaction depends on frequency because of the polarization.

$$V_{\text{eff}}(\omega, q) = \frac{V(q)}{1 + \nu V(q)\displaystyle\int \mathrm{d}\mathbf{n}\,\frac{v_F\mathbf{n}\cdot\mathbf{q}}{v_F\mathbf{n}\cdot\mathbf{q} - \omega - \mathrm{i}0\mathrm{sign}(\omega)}}\,, \tag{4.26}$$

which is called dynamical screening because of the frequency dependence. Other particles will take some time to produce the screening cloud; it does not happen instantaneously. So, it is a retarded process. We will now consider the following limits:

a.) $\omega \mapsto 0$ and $q \ll 2k_F$:

It holds that $\Pi(q) \simeq \nu$ and

$$V_{\text{eff}}(\omega = 0, q) = \frac{V(q)}{1 + \nu V(q)} = \frac{\frac{4\pi e^2}{q^2}}{1 + \nu\frac{4\pi e^2}{q^2}} = \frac{4\pi e^2}{q^2 + \kappa^2}\,, \quad \kappa^2 = 4\pi e^2\nu\,. \tag{4.27}$$

The Fourier transform is given by

$$V_{\text{eff}}(r) = \frac{e^2}{r}\exp(-\kappa r)\,, \tag{4.28}$$

where κ is the inverse **screening length** (Thomas-Fermi screening).

b.) $\omega = 0$ and q arbitrary:

One obtains the Linnhard function, which includes Friedel oscillations. Then, there exists a fast oscillating part, which will oscillate like $1/r^3\cos(2k_F r)$.

c.) $\omega \neq 0$, but small ($\omega \ll qv_F$):

$$\Pi(\omega, q) \simeq \nu\left(1 + \frac{\mathrm{i}\pi}{2}\frac{|\omega|}{v_F q}\right)\,, \tag{4.29}$$

$$V_{\text{eff}}(\omega, q) = \frac{V(q)}{\varepsilon(\omega, q)}\,, \tag{4.30}$$

with the dielectric constant ε. Whenever $\mathrm{Im}(\varepsilon) \neq 0$, it corresponds to dissipation. Whenever there is some excitation, it will be damped under the creation of particle hole pairs ("Landau daming").

d.) $q \mapsto 0$, finite ω

$$\Pi(\omega, q) = -\nu \int \mathrm{d}\mathbf{n} \, \frac{(v_F \mathbf{n} \cdot \mathbf{q})^2}{\omega^2} = -\nu \frac{v_F^2 q^2}{3\omega^2} \,, \tag{4.31}$$

$$\varepsilon(\omega, q) = 1 - \frac{4\pi e^2}{q^2} \nu \frac{v_F^2 q^2}{3\omega^2} = 1 - \left(\frac{\omega_{\mathrm{pl}}}{\omega}\right)^2 \,, \tag{4.32}$$

where

$$\omega_{\mathrm{pl}} = \left(\frac{4\pi}{3} e^2 \nu v_F^2\right)^{\frac{1}{2}} \,, \tag{4.33}$$

is the so-called plasmon frequency. For $\omega = \omega_{\mathrm{pl}}$ it holds that $\varepsilon(\omega, q \mapsto 0) = 0$. The pole in V_{eff} corresponds to excitations, which can propagate. These excitations are bosonic branch effective excitations in the Fermi system with Coulomb interaction and are called plasmons. Plasmons are collective excitations.

Chapter 5

Matsubara Formalism

This chapter deals with a perturbation theory method for $T \neq 0$. A useful book will be AGD Chapter 3

1 1.1. For $T \neq 0$ we replace averages over the ground state by

$$\sum_n \langle n| \exp(\beta(\Omega - \widehat{H} + \mu\widehat{N})|n\rangle \,, \tag{5.1}$$

where $\Omega(T, V, N)$ is the grand canonical potential. It is defined by

$$\Omega = F - \mu N = U - ST - \mu N \,. \tag{5.2}$$

One can change T, S, ... and for example it holds that

$$\mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N \,, \tag{5.3}$$

or

$$\mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - N\,\mathrm{d}\mu \,. \tag{5.4}$$

We will need the Zustandssumme

$$Z_{\mathrm{GC}} = \sum_n \langle n| \exp(-\beta(\widehat{H} - \mu\widehat{N}))|n\rangle = \exp(-\beta\Omega) \,, \tag{5.5}$$

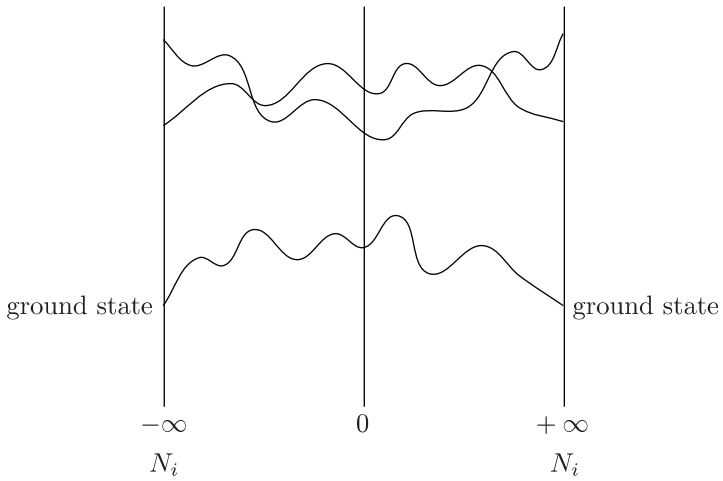
and use the definition

$$\sum_n \langle n| \ldots |n\rangle \equiv \mathrm{Tr}(\ldots) \,. \tag{5.6}$$

Where is now the problem with $T > 0$? At zero temperature we have defined a Green function in the following way:

$$\mathrm{i}G(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \langle|\widehat{S}^{-1} T \widehat{S} \psi_i(\mathbf{r}_1, t_1)\psi_i^\dagger(\mathbf{r}_2, t_2)|0\rangle \,, \tag{5.7}$$

where $|0\rangle$ is the non-interacting ground state. $\widehat{S}$ knows everything about the interaction. The argumentation was $\widehat{S}|0\rangle = \exp(\mathrm{i}\alpha)|0\rangle$. But this also holds for the ground state, because one cannot expect that another state evaluates from $t = -\infty$ to $t = +\infty$ without crossing other levels.



At $T \neq 0$ it holds that

$$\sum_n \langle n| \exp(\beta(\Omega - \widehat{H} - \mu\widehat{N}))\widehat{S}^{-1} T_t(\widehat{S}\widehat{\psi}_i(\mathbf{r}_1, t_1)\widehat{\psi}_i^\dagger(\mathbf{r}_2, t_2)|n\rangle \,. \tag{5.8}$$

Perhaps we can sacrifice the time evolution for states, because this is a complicated object, since it contains the interaction. In thermodynamics we are interested in E, μ, P, ...

5.1 Matsubara Green's function

This is a similar object as G, however with an imaginary time: $\tau \in [0, \beta]$. The motivation is that $\exp(-\beta\widehat{H})$ looks like the time evolution operator $U(-\mathrm{i}\beta)$. We define the Matsubara Green function by

$$\begin{aligned}\mathscr{G}_H(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) &= \\ &= \begin{cases} -\mathrm{Tr}[\exp(\beta(\Omega - \widehat{H} - \mu\widehat{N}))\exp(\widehat{H}(\tau_1 - \tau_2))\psi(\mathbf{r}_1)\exp(-\widehat{H}(\tau_1 - \tau_2))\psi^\dagger(\mathbf{r}_2)] & \text{for} \quad \tau_1 > \tau_2 \\ \pm\mathrm{Tr}[\exp(\beta(\Omega - \widehat{H} - \mu\widehat{N}))\exp(-\widehat{H}(\tau_1 - \tau_2))\psi^\dagger(\mathbf{r}_2)\exp(\widehat{H}(\tau_1 - \tau_2))\psi(\mathbf{r}_1)] & \text{for} \quad \tau_1 < \tau_2 \end{cases},\end{aligned} \tag{5.9}$$

where the plus sign is to be used for fermions and the minus sign for bosons, respectively. $\psi(\mathbf{r}_1)$ and $\psi^\dagger(\mathbf{r}_2)$ are field operators. In the following we will use the notation

$$\mathrm{Tr}[\exp(\beta(\Omega - \widehat{H} - \mu\widehat{N}))] = \langle \ldots \rangle \,, \tag{5.10}$$

and furthermore

$$\psi_{\mathrm{MH}}(\mathbf{r}, \tau) = \exp(\widehat{H}\tau)\psi(\mathbf{r})\exp(-\widehat{H}\tau) \,, \tag{5.11}$$

$$\overline{\psi}_{\mathrm{MH}}(\mathbf{r}, \tau) = \exp(\widehat{H}\tau)\psi^\dagger(\mathbf{r})\exp(-\widehat{H}\tau) \,, \tag{5.12}$$

where $\widehat{H}$ should be understood as $\widehat{H} - \mu\widehat{N}$. The caveat is $\overline{\psi}_{\mathrm{MH}}(\mathbf{r}, \tau) \neq \psi^\dagger_{\mathrm{MH}}(\mathbf{r}, \tau)$. The τ-chronological product is given by

$$T_\tau(\psi_H(1)\overline{\psi}_H(2)) = \begin{cases} \psi_H(1)\overline{\psi}_H(2) & \text{for} \quad \tau_1 > \tau_2 \\ \mp\overline{\psi}_H(2)\psi_H(1) & \text{for} \quad \tau_1 < \tau_2 \end{cases}, \tag{5.13}$$

with $(1) = (\mathbf{r}_1, t_1)$ and $(2) = (\mathbf{r}_2, t_2)$. Finally, we can write up

$$\boxed{\mathscr{G}_M(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) = -\langle T_\tau \psi_H(\mathbf{r}_1, \tau_1)\overline{\psi}_H(\mathbf{r}_2, \tau_2) \,.} \tag{5.14}$$

Remark: Using

$$\widehat{N} = \int \mathrm{d}^3 r \, \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \,, \tag{5.15}$$

one obtains:

$$N = \langle \widehat{N} \rangle = \int \mathrm{d}^3 r \, \langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \rangle = \int \mathrm{d}^3 r \, \mathscr{G}_M(\mathbf{r}, \tau; \mathbf{r}, \tau + 0) \,. \tag{5.16}$$

With $N(\mu, T) \mapsto \mu(n, T)$ with $n = N/V$ one gets

$$\frac{\partial f}{\partial n} = \mu(n, T) \,, \tag{5.17}$$

the free energy density f.

5.1.1 Properties of the Matsubara Green function

1.) From definition it is clear that

$$\mathscr{G}(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) = \mathscr{G}(\mathbf{r}_1, \mathbf{r}_2, \tau = \tau_1 - \tau_2) \,, \tag{5.18}$$

and for homogeneous systems additionally only $\mathbf{r}_1 - \mathbf{r}_2 = \mathbf{r}$ enters.

2.) Let us consider:

$$\Delta\mathscr{G} = \mathscr{G}(\mathbf{r},+0) - \mathscr{G}(\mathbf{r},-0) = -\langle[\psi(\mathbf{r}),\psi^\dagger(0)]_\pm\rangle = -\delta^{(3)}(\mathbf{r})\,, \tag{5.19}$$

hence, $\mathscr{G}$ "jumps" at $\tau = 0$.

3.) $\mathscr{G}(\mathbf{r},\tau)$ is defined for $-\beta < \tau < \beta$, because the object $\exp(\beta(\Omega - \widehat{H} - \mu\widehat{N}))$ must always put to the left due to time-ordering. By using the cyclic invariance of the trace, one obtains:

$$\begin{aligned}
\mathscr{G}(\mathbf{r},\tau<0) &= \pm\mathrm{Tr}(\exp(\beta(\Omega-\widehat{H}-\mu\widehat{N})\exp(-\widehat{H}\tau)\psi^\dagger(\mathbf{r}_2)\exp(\widehat{H}\tau)\psi(\mathbf{r}_1)) = \\
&= \pm\mathrm{Tr}[\exp(\widehat{H}\tau)\psi(\mathbf{r}_1)\exp(\beta(\Omega-\widehat{H}))\exp(-\widehat{H}\tau)\psi^\dagger(\mathbf{r}_2)] = \\
&= \pm\mathrm{Tr}[\exp(\beta\mathrm{i}\Omega)\exp(\widehat{H}\tau)\psi(\mathbf{r}_1)\exp(-\widehat{H}(\tau+\beta))\psi^\dagger(\mathbf{r}_2)] = \\
&= \pm\mathrm{Tr}[\exp(\beta(\Omega-\widehat{H}))\exp(\widehat{H}(\tau+\beta))\psi(\mathbf{r}_1)\exp(-\widehat{H}(\tau+\beta))\psi^\dagger(\mathbf{r}_2)] = \\
&= \mp\mathscr{G}(\mathbf{r},\tau+\beta)\,, \quad \tau+\beta>0\,.
\end{aligned} \tag{5.20}$$

5.2 The Matsubara Green function for free particles

The free Hamiltonian is given by

$$\widehat{H}_0 = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}\,, \tag{5.21}$$

with the dispersion relation

$$\varepsilon_{\mathbf{p}} = \frac{p^2}{2m} - \mu\,. \tag{5.22}$$

The field operators can be written in the form

$$\psi(\mathbf{r}_1) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}_1}\exp(\mathrm{i}\mathbf{p}_1\cdot\mathbf{r}_1)a_{\mathbf{p}_1}\,, \quad \psi^\dagger(\mathbf{r}_2) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}_2}\exp(-\mathrm{i}\mathbf{p}_2\cdot\mathbf{r}_2)^\dagger_{\mathbf{p}_2}\,. \tag{5.23}$$

One obtains:

$$\begin{aligned}
\mathscr{G}_M(\mathbf{r}_1,\mathbf{r}_2,\tau>0) &= -\langle\psi_{\mathrm{MH}}(\tau)\psi(0)\rangle = \\
&= -\frac{1}{V}\sum_{\mathbf{p}_1,\mathbf{p}_2}\exp(\mathrm{i}(\mathbf{p}_1\cdot\mathbf{r}_1-\mathbf{p}_2\cdot\mathbf{r}_2))\times \\
&\quad\times\mathrm{Tr}[\exp(\beta(\Omega-\widehat{H}_0))\exp(\widehat{H}_0\tau)a_{\mathbf{p}_1}\exp(-H_0\tau)a^\dagger_{\mathbf{p}_2})]\exp(-\varepsilon_{\mathbf{p}_1}\tau)a_{\mathbf{p}_1} = \\
&= -\frac{1}{V}\sum_{\mathbf{p}_1,\mathbf{p}_2}\exp(\mathrm{i}(\mathbf{p}_1\cdot\mathbf{r}_1-\mathbf{p}_2\cdot\mathbf{r}_2))\exp(-\varepsilon_{\mathbf{p}_1}\tau)\langle a_{\mathbf{p}_1}a^\dagger_{\mathbf{p}_2}\rangle\,,
\end{aligned} \tag{5.24}$$

with $\langle a_{\mathbf{p}_1}a^\dagger_{\mathbf{p}_2}\rangle \sim \delta_{\mathbf{p}_1\mathbf{p}_2}$, which follows from the orthogonality of states with different quantum numbers. For bosons it holds that

$$\langle a_{\mathbf{p}}a^\dagger_{\mathbf{p}}\rangle = 1 - \langle a^\dagger_{\mathbf{p}}a_{\mathbf{p}}\rangle = 1 - n_{\mathbf{p}}\,, \tag{5.25}$$

with

$$n_{\mathbf{p}} = \frac{1}{\exp(\beta\varepsilon_{\mathbf{p}})+1}\,, \tag{5.26}$$

and for bosons

$$\langle a_{\mathbf{p}}a^\dagger_{\mathbf{p}}\rangle = 1 + n_{\mathbf{p}}\,, \tag{5.27}$$

with

$$n_{\mathbf{p}} = \frac{1}{\exp(\beta\varepsilon_{\mathbf{p}})-1}\,. \tag{5.28}$$

One therefore gets

$$\mathscr{G}_{M,0}(\mathbf{r},\tau>0) = -\frac{1}{V}\sum_{\mathbf{p}}\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})\exp(-\varepsilon_{\mathbf{p}}\tau)(1\mp n_{\mathbf{p}}) \mapsto -\int\frac{\mathrm{d}^3p}{(2\pi)^3}\,\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r})(-\mathscr{G}_{M,0}(\mathbf{p},\tau>0))\,, \tag{5.29}$$

and with $\mathscr{G}_{M,0}(\mathbf{p},\tau>0) = -(1\mp n_{\mathbf{p}})\exp(-\varepsilon_{\mathbf{p}}\tau)$ and

$$\mathscr{G}_{M,0}(\mathbf{p},\tau) = \int \mathrm{d}^3 r\, \exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r})\mathscr{G}_{M,0}(\mathbf{r},\tau)\,, \tag{5.30}$$

for $-\beta<\tau<0$.

$$\begin{aligned}\mathscr{G}_{M,0}(\mathbf{p},\tau<0) = \mathscr{G}_{M,0}(\mathbf{p},\tau+\beta) &= \mp\exp(-\varepsilon_{\mathbf{p}}\tau)\exp(-\varepsilon_{\mathbf{p}}\beta)\left(1\mp\frac{1}{\exp(\varepsilon_{\mathbf{p}}\beta\pm 1)}\right) = \\ &= \mp\exp(-\varepsilon_{\mathbf{p}}\tau)\frac{1}{\exp(\varepsilon_{\mathbf{p}}\beta)\pm 1} = \mp\exp(-\varepsilon_{\mathbf{p}}\tau)n_{\mathbf{p}}\,.\end{aligned} \tag{5.31}$$

5.3 Interaction representation

Like at $T=0$, just write $\mathrm{i}t\mapsto\tau$:

$$\exp(-\widehat{H}\tau) = \exp(-\widehat{H}_0\tau)\mathcal{S}(\tau)\,, \tag{5.32}$$

with $0<\tau<\beta$, $\widehat{H}_0\mapsto\widehat{H}_0-\mu\widehat{N}$, $\widehat{H}=\widehat{H}_0+\widehat{V}$. $\mathcal{S}(\tau)$ is some operator.

$$\psi_{M,0}(\mathbf{r},\tau) = \exp(H_0\tau)\psi(\mathbf{r})\exp(-H_0\tau)\,, \tag{5.33}$$

$$\overline{\psi}_{M,0}(\mathbf{r},\tau) = \exp(H_0\tau)\psi^\dagger(\mathbf{r})\exp(-H_0\tau)\,. \tag{5.34}$$

In particular it holds that

$$\widehat{V}(\tau) = \exp(H_0\tau)\widehat{V}\exp(-H_0\tau)\,. \tag{5.35}$$

Notice $\widehat{H}_0(\tau)=\widehat{H}_0$ and $\widehat{N}(\tau)=\widehat{N}$, because the particle number does not change. The equation of motion for $\mathcal{S}$ is given by

$$-\widehat{H}\exp(-\widehat{H}\tau) = -\widehat{H}\exp(-\widehat{H}_0\tau)\mathcal{S} + \exp(-\widehat{H}_0\tau)\frac{\partial\mathcal{S}}{\partial\tau}\,. \tag{5.36}$$

$$-\exp(H_0\tau)\widehat{H}\exp(-\widehat{H}\tau) + \widehat{H}_0\mathcal{S} = \frac{\partial\mathcal{S}}{\partial\tau}\,, \tag{5.37}$$

The solution of the equation is given by

$$\boxed{\mathcal{S}(\tau) = T_\tau\exp\left(-\int_0^\tau \mathrm{d}\tau'\,\widehat{V}(\tau')\right)\,,} \tag{5.38}$$

$$\boxed{\mathcal{S}(\tau_1,\tau_2) = T_\tau\exp\left(-\int_{\tau_2}^{\tau_1}\mathrm{d}\tau\,\widehat{V}(\tau)\right)\,.} \tag{5.39}$$

Let us look at the properties of $\mathcal{S}$:

$$\mathcal{S}(\tau_1,\tau_3) = \mathcal{S}(\tau_1,\tau_2)\mathcal{S}(\tau_2,\tau_3)\,, \tag{5.40}$$

$$\mathcal{S}(\tau_1,\tau_2) = \mathcal{S}(\tau_1)\mathcal{S}^{-1}(\tau_2)\,. \tag{5.41}$$

$$\psi_{\mathbf{MH}}(\mathbf{r},\tau) = \mathcal{S}^{-1}(\tau,0)\psi_{M,0}(\mathbf{r},\tau)\mathcal{S}(\tau,0)\,, \tag{5.42}$$

for the reason

$$\begin{aligned}\exp(H\tau)\psi\exp(-H\tau) &= \exp(H\tau)\exp(H_0\tau)\exp(-H_0 t)\exp(H_0\tau)\exp(-H_0\tau)\exp(H\tau) = \\ &= \mathcal{S}^{-1}(\tau,0)\mathscr{G}_{M,0}\mathcal{S}(\tau)\,.\end{aligned} \tag{5.43}$$

$$\begin{aligned}\mathscr{G}_M(\tau > 0) &= -\exp(\beta\Omega)\mathrm{Sp}[\exp(-\beta H_0)\mathcal{S}(\beta,\tau_1)\psi_{M,0}(1) + \mathcal{S}(\tau_1,\tau_2)\overline{\psi}_{M,0}(2)\mathcal{S}(\tau_2)] = \\ &= -\exp(\beta(\Omega-\Omega_0))\langle\mathcal{S}(\beta,\tau_1)\psi_{M,0}(1)\mathcal{S}(\tau_1,\tau_2)\overline{\psi}_{M,0}(2)\mathcal{S}(\mathbf{r}_2,0)\rangle_0\,. \end{aligned} \tag{5.44}$$

$$\exp(-\beta\Omega) = \mathrm{Tr}(\exp(-\beta\widehat{H})) = \mathrm{Tr}(\exp(-\beta H_0)\mathcal{S}(\beta))\exp(-\beta\Omega_0)\langle\mathcal{S}\rangle_0 \tag{5.45}$$

$$\boxed{\exp(-\beta(\Omega-\Omega_0)) = \langle\mathcal{S}\rangle_0\,.} \tag{5.46}$$

The final result is given by

$$\boxed{\mathscr{G}_M(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) = -\frac{\langle T_\tau\mathcal{S}\psi(\mathbf{r}_1,\tau_1)\overline{\psi}(\mathbf{r}_2,\tau_2)\rangle_0}{\langle\mathcal{S}\rangle_0}\,,} \tag{5.47}$$

where

$$\langle\ldots\rangle_0 = \mathrm{Sp}(\exp(\beta(\Omega_0 - \widehat{H_0})))\,, \quad \widehat{H}_0 \mapsto \widehat{H}_0 - \mu\widehat{N}\,, \tag{5.48}$$

and

$$\Omega - \Omega_0 = -T\ln(\langle\widehat{S}\rangle_0)\,, \tag{5.49}$$

where $\ln\langle\widehat{S}\rangle_0$ contains the connected vacuum diagrams.

5.4 Wick's theorem at $T \neq 0$

We expand the scattering matrix

$$\widehat{\mathcal{S}} = T_\tau \exp\left(-\int_0^\beta \mathrm{d}\tau\,\widehat{V}(\tau)\right)\,, \tag{5.50}$$

in the interaction:

$$\widehat{\mathcal{S}} = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta \mathrm{d}\tau_1\ldots\int_0^\beta \mathrm{d}\tau_n\,T_\tau\widehat{V}(\tau_1)\ldots\widehat{V}(\tau_n),, \tag{5.51}$$

with

$$\widehat{V} = \frac{1}{2}\int \mathrm{d}r\mathrm{d}r'\,\overline{\psi}(r)\overline{\psi}(r')V(r-r')\psi(r')\psi(r)\,. \tag{5.52}$$

Thus, we need the thermal expectation values

$$\langle T_\tau\psi_{M,0}(\mathbf{r},\tau)\ldots\overline{\psi}_{M,0}(\mathbf{r}',\tau')\rangle\,. \tag{5.53}$$

In a system with $T \neq 0$ the normal ordering concept is no longer useful, because we have no ground state any more. Let us consider

$$H_0 = \sum_\lambda \varepsilon_\lambda a_\lambda^\dagger a_\lambda\,, \tag{5.54}$$

where λ is a quantum number. Eigenstates can be constructed by

$$|n_1,n_2,\ldots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\ldots|0\rangle\,. \tag{5.55}$$

We define

$$\psi_{M,0}(\mathbf{r},\tau) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}}(\tau)\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{r} - \varepsilon_{\mathbf{p}}\tau)\,, \tag{5.56}$$

and

$$\overline{\psi}_{M,0}(\mathbf{r},\tau) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger(\tau)\exp(-\mathrm{i}\mathbf{p}\cdot\mathbf{r} + \varepsilon_{\mathbf{p}}\tau)\,. \tag{5.57}$$

Here, τ was put in $a^\dagger(\tau)$ and $a(\tau)$ for proper time ordering.

$$\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_1}\frac{1}{\sqrt{V}}\sum_{\mathbf{p}_2}\dots\frac{1}{\sqrt{V}}\sum_{\mathbf{p}'_1}\frac{1}{\sqrt{V}}\sum_{\mathbf{p}'_2}\dots\langle T_\tau a_{\mathbf{p}_1}(\tau_1)a_{\mathbf{p}_2}(\tau_2)\dots a^\dagger_{\mathbf{p}'_1}(\tau'_1)a^\dagger_{\mathbf{p}'_2}(\tau'_2)\rangle_0\,, \tag{5.58}$$

with

$$\langle T_\tau a_{\mathbf{p}_1}(\tau_1)a_{\mathbf{p}_2}(\tau_2)\dots a^\dagger_{\mathbf{p}'_1}(\tau'_1)a^\dagger_{\mathbf{p}'_2}(\tau'_2)\rangle_0 = \sum_n\langle n\exp(\beta(\Omega-\widehat{H}_0))a_1a_2\dots a^\dagger a_{1'}a^\dagger a_{2'}\dots|n\rangle_0\,. \tag{5.59}$$

$\langle\dots\rangle_0$ is nonzero only if every $a^\dagger_{\mathbf{p}}$ finds a partner $a_{\mathbf{p}}$. Let us consider the simplest case:

$$T_\tau\underbrace{a_{\mathbf{p}}\underbrace{a_{\mathbf{p}'}a^\dagger_{\mathbf{p}'}}a^\dagger_{\mathbf{p}}}\rangle_0 = \langle T_\tau a_{\mathbf{p}}a^\dagger_{\mathbf{p}}\rangle\langle T_\tau a_{\mathbf{p}'}a^\dagger_{\mathbf{p}'}\rangle\,, \tag{5.60}$$

since the Hamiltonian is a sum of non-correlated sub-Hamiltonians (for $\mathbf{p}\neq\mathbf{p}'$). Averages over different momenta can be done separately. What happens for $\mathbf{p}=\mathbf{p}'$? These terms are suppressed by a factor $1/V$. The rule is as follows:

$$\langle\dots\rangle_0 = \sum_{\substack{\text{contractions over}\\ \text{all possible pairs}}}\langle\dots\rangle\,, \tag{5.61}$$

in the limit $V\mapsto\infty$. The exceptions from this are as follows:

- superconductivity (particle states with momentum $\mathbf{k}$ and hole states with momentum $-\mathrm{k}$ are correlated)
- suprafluidity/Bose-condensation (where $a_0\sim a_0^\dagger\sim\sqrt{N}\sim\sqrt{V}$, holds only for bosons)
- molecules

Therefore, for these cases special techniques are required. Let us consider the following example:

$$\begin{aligned}\langle T_\tau\psi(1)\psi(2)\overline{\psi}(1')\overline{\psi}(2')\rangle_0 &= \langle T_\tau\psi(1)\overline{\psi}(2')\rangle_0\langle T_\tau\psi(2)\overline{\psi}(1')\rangle_0 \mp \langle T_\tau\psi(1)\overline{\psi}(1')\rangle_0\langle T_\tau\psi(2)\overline{\psi}(2')\rangle_0 = \\ &= (-G_{M,0}(1,2'))(-G_{M,0}(2,1')) \mp (-G_{M,0}(1,1'))(-G_{M,0}(2,2'))\,.\end{aligned} \tag{5.62}$$

This indicates, that an expansion in powers of $\mathscr{G}_{M,0}$ and $\widehat{V}$ exists. Comparison between $T=0$ and $T\neq 0$:

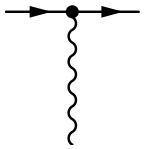
$$\mathscr{G} = -\langle\dots\rangle_0 \qquad \Leftrightarrow \quad G = -\mathrm{i}\langle 0|\dots|0\rangle$$

$$\widehat{\mathcal{S}} = \mathrm{Tr}\left\{\exp\left(-\int\dots\right)\right\} \quad \Leftrightarrow \quad \widehat{S} = T\exp\left(-\mathrm{i}\int\dots\right)$$

$$\int_0^\beta \mathrm{d}\tau\dots \qquad \Leftrightarrow \quad \int_{-\infty}^{+\infty}\mathrm{d}t\dots$$

5.5 Rules of the diagram technique in real space

1.) Write all topologically different connected diagrams with $2n$ vertices



2.) $\mathscr{G}_{M,0}(1,2)$

3.) $V(\mathbf{r}-\mathbf{r}')\delta(\tau_1-\tau_2) = V(1-2)$ (instantaneous interaction)

4.) $\int \mathrm{d}r \int_0^\beta \mathrm{d}\tau$ over all internal coordinates

5.) $(-1)^n(-1)^L$

6.) $\mathscr{G}_{M,0}(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2) \overset{\tau_1\equiv\tau_2}{=} \mathscr{G}_0(\mathbf{r}_1,\mathbf{r}_2,-0)$

7.) spin and symmetry-factors as before at $T=0$

5.6 Matsubara representation

$\mathscr{G}(\tau)$ was defined so far in $-\beta \le \tau < \beta$. The property $\mathscr{G}(\tau<0) = \mp\mathscr{G}(\tau+\beta)$ holds. Formally, one can continue $\mathscr{G}(\tau)$ periodically: $\mathscr{G}(\tau) = \mp\mathscr{G}(\tau+\beta)$ für $\tau \in [-\infty,\infty]$. The Fourier series related τ to ω_n:

$$\mathscr{G}(\tau) = \frac{1}{\beta}\sum_n \exp(-\mathrm{i}\omega_n\tau)\mathscr{G}(\omega_n)\,. \tag{5.63}$$

The coefficients $\mathscr{G}(\omega_n)$ can be obtained by

$$g(\omega_n) = \int_0^\beta \mathrm{d}\tau\, \exp(\mathrm{i}\omega_n\tau)\mathscr{G}(\tau)\,. \tag{5.64}$$

If one chooses $\omega_n = \varepsilon_n = (2n+1)\pi T$, one refers to fermions and with the choice $\omega_n = \nu_n = 2n\pi T$, one refers to bosons (with $\beta^{-1}=T$). This comes from the additional factor $\exp(\mathrm{i}\pi) = -1$ for fermions. Now we come to a remark. At every vertex including fermions and bosons one obtains:

$$\int_0^\beta \mathrm{d}\tau\, \exp\left(\mathrm{i}\tau\left\{\sum_n \varepsilon_n + \sum_n \nu_n\right\}\right) = \beta\delta_{\sum_n \varepsilon_n + \sum_n \nu_n}\,. \tag{5.65}$$

5.7 $\mathscr{G}(\mathbf{p},\varepsilon_n)$ for free particles

The Fourier transform of

$$\mathscr{G}(\mathbf{p},\tau) = -(1\mp n(\mathbf{p}))\exp(-\varepsilon_{\mathbf{p}}\tau)\,, \quad 0<\tau<\beta\,. \tag{5.66}$$

is given by

$$\begin{aligned}\mathscr{G}(\mathbf{p},\omega_n) &= -(1\mp n(\mathbf{p}))\int_0^\beta \mathrm{d}\tau\, \exp(\mathrm{i}\omega_n\tau)\exp(-\varepsilon_{\mathbf{p}}\tau) = \\ &= -(1\mp n(\mathbf{p}))\frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}}\tau}\left[\exp(\mathrm{i}\omega_n\beta)\exp(-\varepsilon_{\mathbf{p}}\beta)-1\right] = \\ &= \frac{1}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}}}\,,\end{aligned} \tag{5.67}$$

using

$$1\mp n(\mathbf{p}) = 1 \mp \frac{1}{\exp(\beta\varepsilon_{\mathbf{p}})\pm 1} = 1 \pm \exp(-\varepsilon_{\mathbf{p}}\beta)\,. \tag{5.68}$$

For **phonons** one can do the same calculation for calculating the photon propagator:

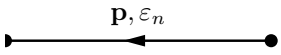
$$D(\mathbf{k},\nu_n) = -\frac{\omega_{\mathbf{k}}^2}{\nu_n^2+\omega_{\mathbf{k}}^2}\,, \quad \omega_{\mathbf{k}} = c|\mathbf{k}|\,. \tag{5.69}$$

5.8 Diagrammatics on momentum frequency domain

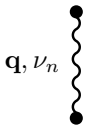
1.) We associate with every line a four-momentum $(\overline{\mathbf{q}}, \omega_n)$ with $\omega_n = \varepsilon_n = (2n+1)\pi T$ for fermions and $\omega_n = \nu_n = 2n\pi T$ for bosons.

2.) Energy-momentum are conserved at every vertex.

3.) $\dfrac{1}{\mathrm{i}\varepsilon_n - \varepsilon_{\mathbf{p}}} \equiv \mathscr{G}_0(\varepsilon_n, \mathbf{p})$



4.) $V(\mathbf{q}, \nu_n) = V(\mathbf{q})$ (because of no retardation at this points)



5.) integration of momenta and frequencies, sum over all internal loops $\displaystyle\prod_i \int \frac{\mathrm{d}^3 p_i}{(2\pi)^3} \frac{1}{\beta} \sum_{n_i}$

6.) $(-1)^n (\mp)^L (2s+1)^L$

Remark: Let us consider the relations between $T = 0$ und $T \neq 0$:

ε, ω $\quad\Leftrightarrow\quad$ ε_n, ν_n with $\varepsilon_n = (2n+1)\pi T$, $\nu_n = 2n\pi T$

$$\int \frac{\mathrm{d}\varepsilon}{2\pi}, \frac{\mathrm{d}\omega}{2\pi} \quad\Leftrightarrow\quad \frac{\mathrm{i}}{\beta}\sum_{\varepsilon_n}, \frac{\mathrm{i}}{\beta}\sum_{\nu_n}$$

Limit $T \downarrow 0$ from Matsubara:

$$\Lambda\varepsilon_n = \varepsilon_{n+1} - \varepsilon_n = 2\pi T\,, \tag{5.70}$$

$$T\sum_{\varepsilon_n} \mapsto \int \frac{\mathrm{d}\varepsilon}{2\pi}\,, \tag{5.71}$$

hence, $\mathscr{G}(0) \overset{T\downarrow 0}{\neq} G(\omega)$.

5.9 Doing sums over Matsubara frequencies

Let us consider

$$n(p) = \langle c_p^\dagger c_p \rangle = \mathscr{G}(\mathbf{p}, -0) = \frac{1}{\beta}\sum_n \frac{1}{\mathrm{i}\varepsilon_n - \varepsilon_{\mathbf{p}}} \exp(\mathrm{i}\varepsilon_n 0)\,. \tag{5.72}$$

The real part of the above sum involves a structure like

$$\frac{1}{\varepsilon_{\mathrm{p}}^2 + \varepsilon_n^2}\,, \quad \varepsilon_n^2 \sim (2n+1)^2\,. \tag{5.73}$$

On can calculate the sum by using a formula in Gradsteyn and Ryshnik:

$$\mathrm{i}\sum_{n=0} \frac{x}{\lambda^2 + \frac{\pi^2}{4}(2n+1)^2} = \tanh(x)\,. \tag{5.74}$$

However, we want to go an alternative way. Let us consider the Fermi function

$$f(z) = \frac{1}{\exp(z\beta) + 1}\,. \tag{5.75}$$

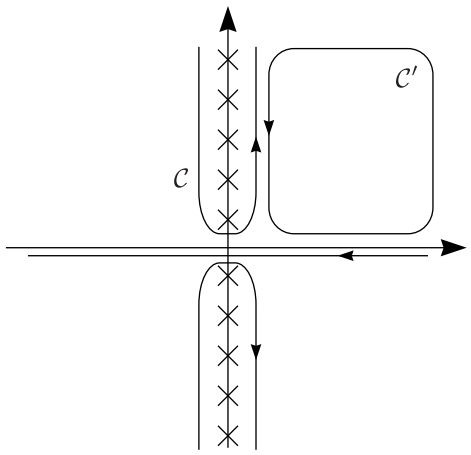
A variable transformation $z = \mathrm{i}\varepsilon_n + \delta$ yields

$$f(\mathrm{i}\varepsilon_n + \delta) = \frac{1}{\exp(\mathrm{i}\varepsilon_n\beta)\exp(\delta\beta) + 1} = \frac{1}{-\exp(\delta\beta) + 1} \sim \frac{1}{-\delta\beta} = \frac{-\frac{1}{\beta}}{\delta}\,. \tag{5.76}$$

So, $f(z)$ has poles on the imaginary axis with the above residues. For a general function $\mathcal{F}(\mathrm{i}\varepsilon_n)$ it holds that

$$\frac{1}{\beta}\sum_n \mathcal{F}(\mathrm{i}\varepsilon_n) = -\oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\,\mathcal{F}(z)f(z)\,. \tag{5.77}$$

with the integration contour $\mathcal{C}$.



$$\int_{\mathcal{C}} = -\int_{\mathcal{C}'}\,, \tag{5.78}$$

if $\mathcal{F}(z)f(z)|z| \mapsto 0$ and $|z| \mapsto \infty$ and if $\mathcal{F}(z)$ has its poles along the real axis.

$$\frac{1}{\beta}\sum_n \mathcal{F}(\mathrm{i}\varepsilon_n) = -\oint_{\mathcal{C}'} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\mathcal{F}(z)f(z)\,, \quad \mathcal{F}(z) = \frac{1}{z - \varepsilon_{\mathbf{p}}}\exp(z\cdot 0)\,, \tag{5.79}$$

and

$$n_{\mathbf{p}} = -\oint_{\mathcal{C}'} \frac{\mathrm{d}z}{2\pi\mathrm{i}}\frac{\exp(z\cdot 0)}{z - \varepsilon_{\mathbf{p}}}f(z) = f(\varepsilon_{\mathbf{p}})\,. \tag{5.80}$$

One can repeat the same for bosons:

$$f(z) \mapsto g(z) = \frac{1}{\exp(\beta z) - 1}\,. \tag{5.81}$$

Hence, the result is:

$$\frac{1}{\beta}\sum_n \frac{\exp(\mathrm{i}\omega_n\cdot 0)}{\mathrm{i}\nu_n - x} = \pm\frac{1}{\exp(\beta x)\pm 1}\,. \tag{5.82}$$

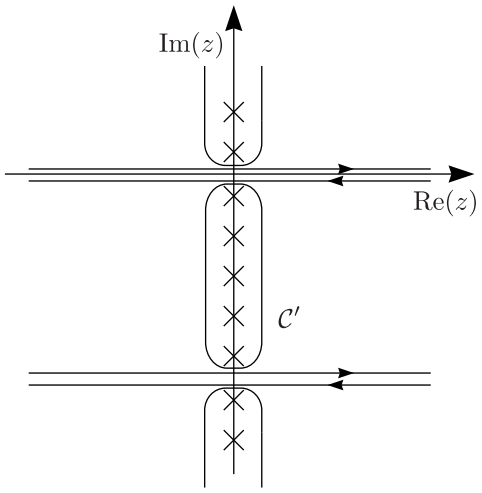
5.9.1 Polarization

$$\Pi(q,\nu_n) = \quad = (-1)\cdot 2\int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{1}{\beta}\sum_{\varepsilon_n}\mathscr{G}(p+q,\varepsilon_n+\nu_n)\mathscr{G}_0(p,\varepsilon_n) \tag{5.83}$$

p, ε_n

$p+q, \varepsilon_n + \nu_n$

$$\frac{1}{\beta}\sum_{\varepsilon_n}\mathscr{G}(p+q,\varepsilon_n+\nu_n)\mathscr{G}_0(p,\varepsilon_n) = -\oint_{\mathcal{C}'}\frac{\mathrm{d}z}{2\pi\mathrm{i}}\,\frac{1}{z+\mathrm{i}\nu_n - \varepsilon_{\mathbf{p}+\mathbf{q}}}\frac{1}{z-\varepsilon_{\mathbf{p}}}f(z)\,. \tag{5.84}$$



$$\frac{f(\varepsilon_{\mathbf{p+q}} - \mathrm{i}\nu_n)}{\varepsilon_{\mathbf{p+q}} - \mathrm{i}\nu_n - \varepsilon_{\mathbf{p}}} + \frac{f(\varepsilon_{\mathbf{p}})}{\varepsilon_{\mathbf{p}} + \mathrm{i}\nu_n - \varepsilon_{\mathbf{p+q}}} \tag{5.85}$$

$$f(x + \mathrm{i}\nu_n) = \frac{1}{\exp(\beta x)\exp(\mathrm{i}\beta\nu_n) + 1} = f(x)\,. \tag{5.86}$$

$$\Pi(q, \nu_n) = 2\int \frac{\mathrm{d}^3 p}{(2\pi)^3}\, \frac{f(\varepsilon_{\mathbf{p+q}}) - f(\varepsilon_{\mathbf{p}})}{\mathrm{i}\nu_n - (\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}})}\,. \tag{5.87}$$

5.10 Time-dependent Green functions at $T \neq 0$

$$\mathscr{G}(\mathbf{r}, \tau; \beta N) = -\mathrm{Tr}\left\{\exp(\beta(\Omega - \widehat{H}))T_\tau \psi_{MH}(\mathbf{r}, \tau)\overline{\psi}_{MH}(0,0)\right\}\,, \tag{5.88}$$

$$G(\mathbf{r}, t; \beta N) = -\mathrm{iTr}\left\{\exp(\beta(\Omega - \widehat{H}))T_t \psi_H(\mathbf{r}, t)\psi_H^\dagger(0,0)\right\}\,. \tag{5.89}$$

We use the Lehmann representation to show that $G(\mathbf{p}, \omega)$ is not analytic in ω. Introduce G^R, G^A, which are analytic in the upper or lower half-plane.

$$G^R(\mathbf{p}, \omega) = \mathrm{Re}(G(\mathbf{p}, \omega)) + \mathrm{iIm}(G(\mathbf{p}, \omega))\left(\coth\left(\frac{\beta\omega}{2}\right)\right)^{\pm 1}\,, \tag{5.90}$$

$$G^A(\mathbf{p}, \omega) = \mathrm{Re}(G(\mathbf{p}, \omega)) - \mathrm{iIm}(G(\mathbf{p}, \omega))\left(\coth\left(\frac{\beta\omega}{2}\right)\right)^{\pm 1}\,, \tag{5.91}$$

where the plus-sign stands for fermions and the minus-sign for bosons. Formal definition:

$$G^R(\mathbf{r}, t) = \begin{cases} -\mathrm{iTr}\left(\exp(\beta(\Omega - \widehat{H}))[\psi(\mathbf{r}, t), \psi^\dagger(0,0)]_\pm\right) & \text{für} \quad t > 0 \\ 0 & \text{für} \quad t < 0 \end{cases}\,, \tag{5.92}$$

$$G^A(\mathbf{r}, t) = \begin{cases} 0 & \text{für} \quad t > 0 \\ \mathrm{iTr}\left(\exp(\beta(\Omega - \widehat{H}))[\psi(\mathbf{r}, t), \psi^\dagger(0,0)]_\pm\right) & \text{für} \quad t < 0 \end{cases}\,. \tag{5.93}$$

Lehmann-representation:

$$G^R(\mathbf{p}, \omega) = \int_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{\varrho(\mathbf{p}, \omega')}{\omega' - \omega - \mathrm{i}0}\,, \quad G^A(\mathbf{p}, \omega) = \int \mathrm{d}\omega'\, \frac{\varrho(\mathbf{p}, \omega')}{\omega' - \omega + \mathrm{i}0} = (G^R(\mathbf{p}, \omega))^*\,. \tag{5.94}$$

$$\varrho(\mathbf{p}, \omega) = -\sum_{n,m} \exp(\beta\Omega)\left(\exp(-\beta E_n \pm \exp(-\beta E_m))\right)|\langle n|\psi(\mathbf{r} = \mathbf{o})|m\rangle|^2 \times \\ \times (2\pi)^3 \delta(\mathbf{p} - (\mathbf{p} - \mathbf{p}_n))\delta(\omega - (E_m - E_n))\,, \tag{5.95}$$

where it holds that

$$\langle n|\psi(\mathbf{r})|m\rangle = \exp(-\mathrm{i}(\mathbf{p}_n - \mathbf{p}_m)\cdot\mathbf{r})\langle m|\psi(\mathbf{o})|n\rangle\,, \tag{5.96}$$

due to translational invariance.

$$G(\omega,\mathbf{p}) = \mathrm{Re}(G^R(\mathbf{p},\omega)) + \left\{ \begin{array}{c} \mathrm{i}\tanh\left(\frac{\omega}{2T}\right) \\ \mathrm{i}\coth\left(\frac{\omega}{2T}\right) \end{array} \right\} \mathrm{Im}(G^R(\mathbf{p},\omega))\,. \tag{5.97}$$

Using the same arguments now for $\mathscr{G}$ yields

$$\mathscr{G}(\mathbf{p},\omega_n) = \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega'\, \frac{\varrho(\mathbf{p},\omega')}{\omega' - \mathrm{i}\omega_n}\,. \tag{5.98}$$

with the same spectral function. The consequences are as follows: $g(\omega_n) = G^R(\mathrm{i}\nu_n)$ für all $\omega_n > 0$ and $g(-\omega_n) = g^*(\omega_n)$. Furthermore it holds that $g(\omega_n) = G^R(\mathrm{i}\omega_n)$ for $\omega_n < 0$. Analytical continuation: Assume, we find an analytical function $\mathcal{F}(z)$, such that $\mathcal{F}(\mathrm{i}\omega_n) = g(\omega_n)\ \forall\ \omega_n > 0$. Hence, an analytical continuation will be $\mathcal{F}(\omega) = G^R(\omega)$ for $\mathrm{Im}(\omega) > 0$.

5.10.1 Linear response at $T \neq 0$ (higher correlation functions)

$$\mathscr{D}_{BA}(\tau) = -\langle T_\tau \widehat{B}(\tau)\widehat{A}(\tau)\rangle\,, \quad \langle\ldots\rangle = \mathrm{Tr}[\exp(\beta(\Omega - \widehat{H}))]\,. \tag{5.99}$$

The operators $\widehat{A}$ and $\widehat{B}$ will be in a Heisenberg representation. For instance, $\widehat{B}$ could be the density operator $\widehat{n}(\mathbf{r})$ and $\widehat{A}$ the density operator $\widehat{n}(\mathbf{r}')$ at a different point $\mathbf{r}'$. Strategy: Calculate $\mathscr{D}_{BA}(\nu_n)$ and then try to find $\mathcal{F}(z)$, such that $\mathcal{F}(\mathrm{i}\nu_n) = \mathscr{D}_B(\nu_n)\ \forall\ \nu_n > 0$. Example:

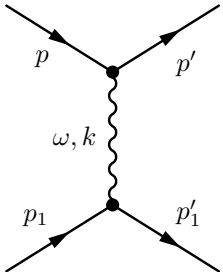
$$\Pi(\mathbf{q},\nu_n) = 2\int \frac{\mathrm{d}^3p}{(2\pi)^3}\, \frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}}) - f(\varepsilon_{\mathbf{p}})}{\mathrm{i}\nu_n - (\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}})}\,, \tag{5.100}$$

$$\Pi^R(\mathbf{q},\omega) = \mathrm{i}\int \frac{\mathrm{d}^3p}{(2\pi)^3}\, \frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}}) - f(\varepsilon_{\mathbf{p}})}{\omega - \varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_{\mathbf{p}} + \mathrm{i}0}\,. \tag{5.101}$$

Chapter 6

Superconductivity

6.1 Cooper instability of a Fermi liquid with attractive interactions



The interaction is mediated by phonons.

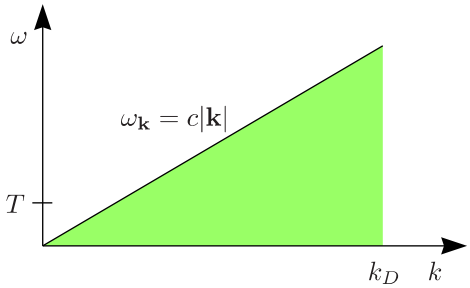
$$\widehat{H}_{\rm int} = g \int {\rm d}^3 r \, \widehat{\psi}^\dagger(\mathbf{r}) \widehat{\psi}(\mathbf{r}) \widehat{\varphi}(\mathbf{r}) \,, \tag{6.1}$$

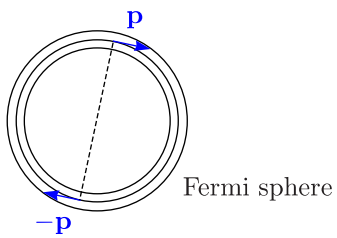
with the propagator of the phonons

$$D(\mathbf{r},t) = -{\rm i}\langle \Phi_0 | T \widehat{\varphi}(\mathbf{r},t) \widehat{\varphi}(0,0) | \Phi_0 \rangle \,, \quad D(k,\omega) = \frac{\omega_k^2}{\omega^2 - \omega_k^2 + {\rm i}0} \,, \quad \omega_k = c|\mathbf{k}| \,. \tag{6.2}$$

If one integrates out the phonons, one gets an effective interaction

$$V_{\rm eff}(k,\omega) = g^2 \frac{\omega_k^2}{\omega^2 - \omega_k^2 + {\rm i}0} \,. \tag{6.3}$$





Exchange processes take place with electrons that are sitting in the vicinity of the Fermi sphere. During such a process one electron gains and the other one looses energy, whereas the energy exchange is very small, but the momentum exchange is large. Hence, we will look at processes, in which particles sit in the opposite site of the Fermi sphere. The condition that needs to be fulfilled by an electron pair to attract is $p + p_1 \approx 0$. Hence, the scattering process that we want has the property that two particles are created and annihilated simultaneously.

$$C = -{\rm i}\langle T\psi(x)\psi(x)\psi^\dagger(0)\psi^\dagger(0)\rangle \,, \quad x = (r,t) \,. \tag{6.4}$$

The bare correlator looks like a bubble, with two times a propagator that starts at $(0,0)$ and go to (x,t). Let us calculate the first elementary diagram and see how to incorporate the interaction.

$$C^{(0)}(q,\omega) = -{\rm i}(-1) \int \frac{{\rm d}\varepsilon}{2\pi} \int \frac{{\rm d}^d p}{(2\pi)^d} \, G\left(\varepsilon + \frac{\omega}{2}, p + \frac{q}{2}\right) G\left(-\varepsilon + \frac{\omega}{2}, -p + \frac{q}{2}\right) \,. \tag{6.5}$$

We introduce

$$\xi = \frac{p^2}{2m} - \mu\,, \quad \int \frac{\mathrm{d}^d p}{(2\pi)^d} \mapsto \nu_F \int \mathrm{d}\xi \int \mathrm{d}n\,, \tag{6.6}$$

and obtain (where terms $\mathbf{O}(q^2)$ are dropped):

$$C^{(0)} = \mathrm{i}\nu \int \mathrm{d}\xi \int \mathrm{d}n \int \frac{\mathrm{d}\varepsilon}{2\pi} \frac{1}{\varepsilon + \frac{\omega}{2} - \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} + \mathrm{i}0\mathrm{sign}\left(\frac{\xi + v_F \mathbf{n}\cdot\mathbf{q}}{2}\right)} \times$$
$$\times \frac{1}{-\varepsilon + \frac{\omega}{2} - \xi + \frac{v_F \mathbf{n}\cdot\mathbf{q}}{2} + \mathrm{i}0\mathrm{sign}\left(\xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2}\right)}\,. \tag{6.7}$$

We wan use the residue theorem. We are only interested in the two cases where the poles sit on different sites. In the first case

$$\xi + v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} > 0\,, \quad \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} > 0\,, \tag{6.8}$$

holds and we close the contour in the lower half plane. In the second case

$$\xi + v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} < 0\,, \quad \xi - v_F \frac{\mathbf{n}\cdot\mathbf{q}}{2} < 0\,, \tag{6.9}$$

holds and we close the contour in the upper half plane. We then obtain the result

$$\nu \int\limits_1 \mathrm{d}\xi \int \mathrm{d}n \, \frac{-1}{2\xi - \omega + \mathrm{i}0} + \int\limits_2 \mathrm{d}\xi \int \mathrm{d}n \, \frac{1}{2\xi - \omega - \mathrm{i}0}\,. \tag{6.10}$$

Now, consider the case $|\xi| > |\omega|$, $|v_F \mathbf{n}\cdot\mathbf{q}$: This leaves us with

$$\int\limits_{\max(|\omega|, |v_F \mathbf{n}\cdot\mathbf{q}|)}^{\varepsilon^*} \frac{\mathrm{d}\xi}{|\xi|}\,. \tag{6.11}$$

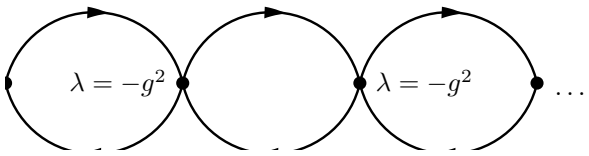
So we run into some singularity, which is cut-off by frequency or wave number.

$$C^{(0)}(q,\omega) \simeq -\nu \ln\left(\frac{\varepsilon^*}{\max(|\omega|, |v_F \mathbf{n}\cdot\mathbf{q}|)}\right)\,. \tag{6.12}$$

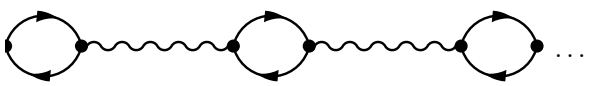
Here, the ξ-cutoff is given by the Fermi energy ε_F. We make a sketch that shows, how to treat a logarithmic singularity. We consider the "ladder diagrams" The interaction shall look like $V(\omega, q) \simeq -g^2$. Then in real space it is a local interaction

$$V(\mathbf{r}, \mathbf{r}'; t, t') = -g^2 \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')\,, \tag{6.13}$$

and our ladder diagrams can be drawn as



Recall RPA, where we summed up a series of the form



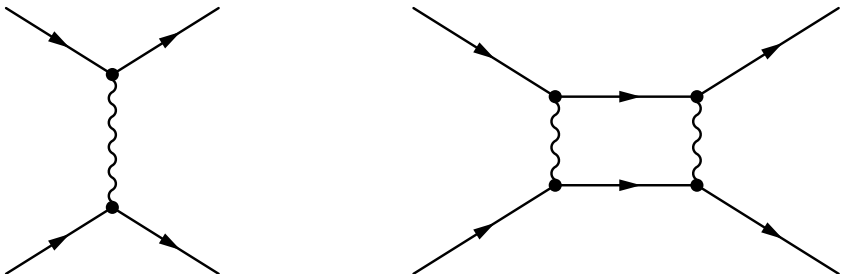
The above summation can be done in an analogous way and we obtain

$$C(q,\omega) = \frac{C^{(0)}(q,\omega)}{1 - \lambda C^{(0)}(q,\omega)}\,, \quad C(q,\omega) = \frac{\nu \ln\left(\frac{\varepsilon^*}{\omega}\right)}{1 + \lambda\nu \ln\left(\frac{\varepsilon^*}{\omega}\right)}\,. \tag{6.14}$$

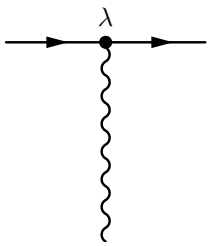
The summation of the ladder diagrams has solves the singularity problem. However, there is a new singularity, which comes into the game, namely when the denominator is zero. When this is the case, something collective is going on that leads to the break down of ground state, which was used for perturbation theory ("Stoner instability").

$$\omega \simeq \varepsilon^* \exp\left(-\frac{1}{|\lambda| v}\right) . \tag{6.15}$$

For $\lambda > 0$ there is, of course, no singularity, but for $\lambda < 0$ (attractive interaction). The instability indicates (in analogy with magnetism) that $\langle T\psi_\uparrow \psi_\downarrow \rangle$, $\langle T\psi_\uparrow^\dagger \psi_\downarrow^\dagger \rangle$ are not zero (when the number of particles in the ground state can fluctuate). This happens, when the Fermi system loses particles that pair and create bosons. In point from the Fermi liquid these particles are lost. Remark: For the nature of the bound states the scattering amplitude should be calculated. The ladder summation



tells us that the bare vertex



goes to

$$\Gamma(\omega) = \frac{\lambda}{1 + \lambda \nu \ln\left(\frac{\varepsilon^*}{\omega}\right)} , \tag{6.16}$$

which indicates are large attraction, when the denominator goes to zero.

6.2 BCS theory

We consider the Hamiltonian

$$\widehat{H} = \sum_{p,\alpha} \xi_p a_{p,\alpha}^\dagger a_{p,\alpha} + \frac{1}{2} \sum_{\substack{p+p'=q+q' \\ \alpha,\beta}} V_{p,p',q',q} a_{p,\alpha}^\dagger a_{p',\beta}^\dagger a_{q,\beta} a_{q,\alpha} , \tag{6.17}$$

with

$$V_{p,p',q,q'} = \frac{1}{V} \begin{cases} \lambda & \text{for} \quad |\xi_{\max}| < \omega_D \\ 0 & \text{else} \end{cases} \quad , \quad |\xi_{\max}| = \max(|\xi_p|, |\xi_{p'}|, |\xi_q|, |\xi_{q'}|) , \quad \xi_p = v_F(p - p_F) . \tag{6.18}$$

Only such electrons interact with each other that sit in a very narrow shell at the Fermi energy. We keep only pairs with $p' = -p$, $q' = -q$. So, only particles that live on the other side of the Fermi surface, will interact with each other. We introduce a field

$$\widehat{B}_{\alpha,\beta}^\dagger = \sum_p a_{p,\alpha}^\dagger a_{-p,\beta}^\dagger . \tag{6.19}$$

The expectation value of this operator is

$$\Delta^* = \frac{\lambda}{V} \sum_p \langle a_{p,\uparrow}^\dagger a_{-p,\downarrow}^\dagger \rangle , \tag{6.20}$$

$$\Delta = \frac{\lambda}{V} \sum_p \langle a_{p,\downarrow}, a_{-p,\uparrow} \rangle \,. \tag{6.21}$$

Now, the means field Hamiltonian looks like

$$\widehat{H} = \sum_p \xi_p (a^\dagger_{p,\uparrow} a_{p,\uparrow} + a^\dagger_{p,\downarrow} a_{p,\downarrow}) + \sum_p \left(\Delta a^\dagger_{p,\downarrow} a^\dagger_{-p,\uparrow} + \Delta^* a_{p,\uparrow} a_{-p,\downarrow} \right) . \tag{6.22}$$

Let us diagonalize the Hamiltonian by introducing

$$c_{p,\uparrow} = u_p a_{p,\uparrow} + v_p a^\dagger_{-p,\downarrow} \,, \quad c_{p,\downarrow} = u_p a_{p,\downarrow} - v_p a^\dagger_{-p,\downarrow} \,. \tag{6.23}$$

Determine u_p, $v_p \in \mathbb{C}$ so that

$$\widehat{H} = E_0 + \sum_{p,\alpha} \varepsilon_p c^\dagger_{p,\alpha} c_{p,\alpha} \,. \tag{6.24}$$

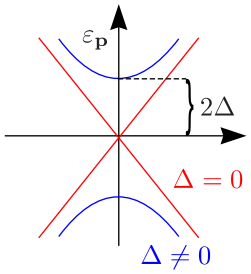
The result is

$$u_p^2 = \frac{1}{2} \left(1 + \frac{\xi_p}{\varepsilon_p} \right) , \quad v_p^2 = \frac{1}{2} \left(1 - \frac{\xi_p}{\varepsilon_p} \right) , \tag{6.25}$$

with

$$\varepsilon_p = (\xi_p^2 + \Delta^2)^{\frac{1}{2}} \,, \quad \Delta \in \mathbb{R} \,. \tag{6.26}$$

Hence, one obtains a change in the dispersion relation, namely an energy gap.



Plugging

$$a_{p,\uparrow} = u_p c_{p,\uparrow} - v_{p'} c^\dagger_{-p,\downarrow} \,, \quad a_{p,\downarrow} = u_p c_{p,\downarrow} + v_p c^\dagger_{-p,\uparrow} \,, \tag{6.27}$$

in the definition of Δ one obtains a self-consistency equation

$$\Delta = \frac{|\lambda|}{V} \sum_p \frac{\Delta}{2(\xi_p^2 + \Delta^2)^{\frac{1}{2}}} \,, \quad 1 = \frac{|\lambda|}{V} \sum_p \frac{1}{2(\xi_p^2 + \Delta^2)^{\frac{1}{2}}} \,. \tag{6.28}$$

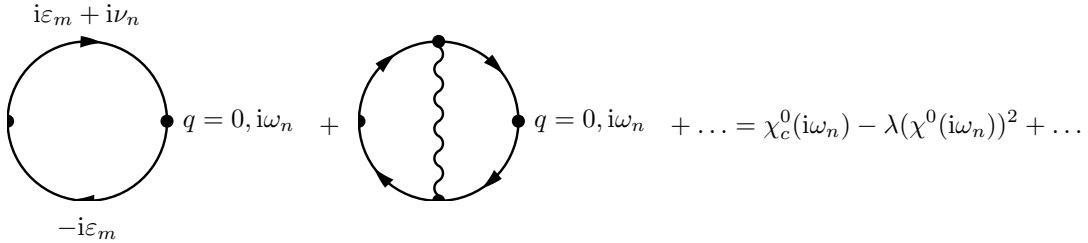
We replace the summation by an integral

$$1 = \frac{|\lambda|}{2} \nu \int_{-\omega_D}^{\omega_D} \mathrm{d}\xi \, \frac{1}{(\xi^2 + \Delta^2)^{\frac{1}{2}}} \,, \tag{6.29}$$

and we obtain the answer

$$\boxed{\Delta \approx \omega_D \exp\left(-\frac{1}{|\lambda| \nu} \right) .} \tag{6.30}$$

Remark:

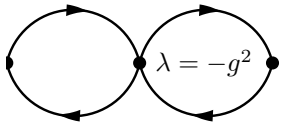


(6.31)

Since the interaction is of the form

$$V_{\text{eff}}(\mathbf{r},\mathbf{r}';t,t') \sim g\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,, \tag{6.32}$$

one can consider the diagram



instead of

Then, one obtains an additional minus sign in the second summand. Summing all contributions yields

$$\chi_c(\mathrm{i}\omega_n) = \frac{\lambda_c^{(0)}(\mathrm{i}\omega_n)}{1+\lambda\chi_c^{(0)}(\mathrm{i}\omega_n)}\,, \quad \chi_c^{(0)}(\mathrm{i}\omega_n) = \sum_m \int \mathrm{d}\xi\, \frac{T\nu}{\mathrm{i}\varepsilon_m + \mathrm{i}\omega_n - \xi}\frac{1}{-\mathrm{i}\varepsilon_m - \xi}\,, \tag{6.33}$$

with

$$\varepsilon_m = (2m+1)\pi T\,, \tag{6.34}$$

for fermions and

$$\omega_n = 2n\pi T\,, \tag{6.35}$$

for bosons. Let $\omega_n = 0$.

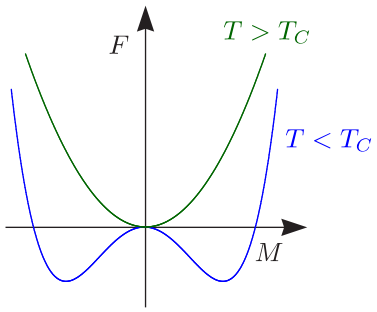
$$\chi_c^{(0)}(\mathrm{i}\omega_n = 0) = T\sum_m \nu \int \mathrm{d}\xi\, \frac{1}{\varepsilon_n^2+\xi^2} = \nu \int_{-\omega_D}^{\omega_D} \mathrm{d}\xi\, \frac{1}{2\xi}\tanh\left(\frac{\xi}{2T}\right) = \nu \ln\left(\frac{\omega_D}{T}\frac{2\gamma}{\pi}\right)\,, \tag{6.36}$$

where $\ln\gamma = c \approx 0,577$ is the Euler constant. ω_D has been chosen as a cut-off, because the interaction is carried out by phonons. If one cools below the temperature

$$T_C = \frac{2\gamma}{\pi}\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right)\,, \tag{6.37}$$

the system becomes instable and there will be a phase transition.

6.3 Remark on spontaneous symmetry breaking



If one goes below the temperature T_c the magnet has to make up its mind, in which direction to point. There will be now domain walls, because they are energetically cost-intensive. Rotating the magnetization around some action does not cost any energy. Which direction it picts, depends on many thing as for example the boundary conditions. Therefore, rotation symmetry O(3) will be broken. If one direction is preferred, the

symmetry O(2) remains. A transformation under this remaining symmetry group does not cost much energy. This is the reason, why waves (magnons) can emerge that respect this symmetry and these waves correspond to massless excitations, so-called Goldstone bosons.
The superconductor also has spontaneous symmetry breaking. This can be understood as follows. A Hamiltonian $H = \psi^\dagger\psi$ is invariant under the operation $\psi \mapsto \psi\exp(\mathrm{i}\varphi)$. So is the Hamiltonian $H = \psi^\dagger\psi^\dagger\psi\psi$. However, the ground state that corresponds to a non-zero value of the expectation value $\langle a_{p,\uparrow}a_{-p,\downarrow}\rangle$, is not invariant under such a U(1) transformation. Hence, the symmetry is spontaneously broken.

6.4 Green function in a superconductor

We consider

$$G_{\alpha\beta}(1,2) = -\mathrm{i}\langle T\psi_\alpha(1)\psi^\dagger_\beta(2)\rangle\,, \tag{6.38}$$

$$F_{\alpha\beta}(1,2) = -\mathrm{i}\langle T\psi_\alpha(1)\psi_\beta(2)\rangle\,, \tag{6.39}$$

and

$$\overline{F}_{\alpha\beta}(1,2) = -\mathrm{i}\langle T\psi^\dagger_\alpha(1)\psi^\dagger_\beta(2)\rangle\,. \tag{6.40}$$

We use the equation of motion method for Green functions and write down the Hamiltonian

$$\widehat{H} = \int \mathrm{d}r\,\left\{\psi^\dagger_\alpha\left(-\frac{p^2}{2m}-\mu\right)\widehat{\psi}_\alpha + \frac{\lambda}{2}(\widehat{\psi}^\dagger_\alpha\widehat{\psi}^\dagger_\alpha)(\widehat{\psi}^\dagger_\gamma\widehat{\psi}_\gamma)\right\}\,. \tag{6.41}$$

We derive the equations of motion for $\widehat{\psi}$ by using

$$\mathrm{i}\frac{\partial}{\partial t}\widehat{\psi} = [\widehat{\psi},\widehat{H}]\,, \tag{6.42}$$

and obtain

$$\mathrm{i}\frac{\partial}{\partial t}\widehat{\psi}_\alpha(x) = -\left(\frac{\boldsymbol{\nabla}^2}{2m}+\mu\right)\widehat{\psi}_\alpha(x) + \lambda\widehat{\psi}^\dagger_\gamma(x)\widehat{\psi}_\gamma(x)\widehat{\psi}_\alpha(x)\,, \tag{6.43}$$

and

$$\mathrm{i}\frac{\partial}{\partial t}\widehat{\psi}^\dagger_\alpha(x) = \left(\frac{\boldsymbol{\nabla}^2}{2m}+\mu\right)\widehat{\psi}^\dagger_\alpha(x) - \lambda\widehat{\psi}^\dagger_\gamma(x)\widehat{\psi}_\gamma(x)\widehat{\psi}^\dagger_\alpha(x)\,. \tag{6.44}$$

One obtains the equations of motion for the Green function by multiplying with $-\mathrm{i}\psi^\dagger(x')$ and doing the average $\langle T\ldots\rangle$ and one finally gets

$$\left(\mathrm{i}\frac{\partial}{\partial t}+\frac{\boldsymbol{\nabla}}{2m}+\mu\right)G_{\alpha\beta}(x,x') + \mathrm{i}\lambda\langle T\widehat{\psi}^\dagger_\gamma(x)\widehat{\psi}_\gamma(x)\widehat{\psi}_\alpha(x)\widehat{\psi}^\dagger_\beta(x')\rangle = \delta_{\alpha\beta}\delta(x-x')\,. \tag{6.45}$$

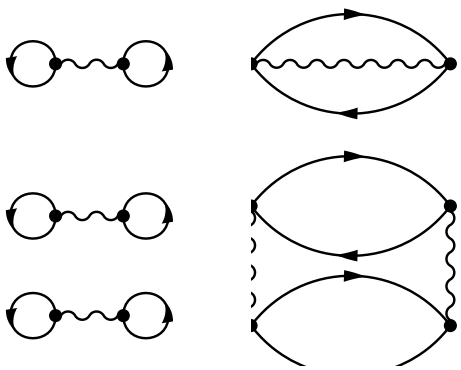
The idea is to replace

$$\langle T\widehat{\psi}^\dagger_\gamma(x)\widehat{\psi}_\gamma(x)\widehat{\psi}_\alpha(x)\widehat{\psi}^\dagger_\beta(x')\rangle\,, \tag{6.46}$$

by

$$\langle T\psi_\gamma(x)\psi_\alpha(x)\rangle\langle T\psi^\dagger_\gamma(x)\psi^\dagger_\beta(x')\rangle\,, \tag{6.47}$$

because we do mean-field theory. We forget the other contributions



because they only contribute to the density of the system and to a change of the chemical potential. Now, we obtain

$$\mathrm{i}^2 F_{\mu\alpha}(x,x)\overline{F}_{\gamma\beta}(x,x')\,. \tag{6.48}$$

The spin structure is $G_{\alpha\beta} \sim \delta_{\alpha\beta}$ and

$$F_{\alpha\beta},\, \overline{F}_{\alpha\beta} \sim g_{\alpha\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{6.49}$$

since they combine spin up with spin down. Hence, one can write $F_{\alpha\beta} = F g_{\alpha\beta}$ etc. It holds that

$$\sum_\gamma g_{\gamma\alpha} g_{\gamma\beta} = \delta_{\alpha\beta}\,. \tag{6.50}$$

$$\boxed{\left(\mathrm{i}\frac{\partial}{\partial t} + \frac{\boldsymbol{\nabla}^2}{2m} + \mu\right) G(x-x') - \mathrm{i}\lambda F(0)\overline{F}(x-x') = \delta(x-x')\,.} \tag{6.51}$$

(translational invariance) Analogously, for F and $\overline{F}$ one obtains

$$\boxed{\left(\mathrm{i}\frac{\partial}{\partial t} - \frac{\boldsymbol{\nabla}^2}{2m} - \mu\right) \overline{F}(x-x') + \mathrm{i}\lambda\overline{F}(0) G(x-x') = 0\,.} \tag{6.52}$$

$$F(0) = -\mathrm{i}\langle\psi_\uparrow(x)\psi_\downarrow(x)\rangle\,, \quad \overline{F}(0) = -\mathrm{i}\langle\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\rangle = F^*(0)\,. \tag{6.53}$$

Fourier transformation yields

$$(\varepsilon - \xi_p) G(\varepsilon,p) - \mathrm{i}\lambda F(0)\overline{F}(\varepsilon,p) = 1\,, \tag{6.54}$$

and

$$(\varepsilon + \xi_p)\overline{F}(\varepsilon,p) + \mathrm{i}\lambda F^*(0) G(\varepsilon,p) = 0\,. \tag{6.55}$$

One the obtains

$$G(\varepsilon,p) = \frac{\varepsilon + \xi_p}{\varepsilon^2 - \xi_p^2 - \Delta^2}\,, \quad \Delta^2 = \lambda^2 |\widetilde{F}(0)|^2\,. \tag{6.56}$$

We decompose the object into two propagators

$$-\frac{u_p^2}{\varepsilon - \varepsilon_p} + \frac{v_p^2}{\varepsilon + \varepsilon_p}\,, \quad u_p^2 = \frac{1}{2}\left(1 + \frac{\xi_p}{\varepsilon_p}\right), \quad v_p^2 = \frac{1}{2}\left(1 - \frac{\xi_p}{\varepsilon_p}\right), \tag{6.57}$$

and

$$\varepsilon_p = (\xi_p^2 + \Delta^2)^{\frac{1}{2}}\,. \tag{6.58}$$

Now, we can introduce the pole structure by adding $+\mathrm{i}0$ for $\varepsilon > 0$ and $-\mathrm{i}0$ for $\varepsilon < 0$:

$$\boxed{G(\varepsilon,p) = \frac{\varepsilon + \xi_p}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i})}\,.} \tag{6.59}$$

$$\overline{F}(\varepsilon,p) = -\mathrm{i}\lambda \frac{F^*(0)}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i}0)}\,. \tag{6.60}$$

By plugging in

$$F^*(0) = \int \frac{\mathrm{d}\varepsilon}{2\pi} \frac{\mathrm{d}^3 p}{(2\pi)^3}\, \overline{F}(\varepsilon,p)\,, \tag{6.61}$$

one obtains the equation

$$1 = \mathrm{i}\lambda \int \frac{\mathrm{d}\varepsilon\, \mathrm{d}^3 p}{(2\pi)^4}\, \frac{1}{(\varepsilon - \varepsilon_p + \mathrm{i}0)(\varepsilon + \varepsilon_p - \mathrm{i}0)}\,. \tag{6.62}$$

Solve this gap equation (as we did before) and obtain

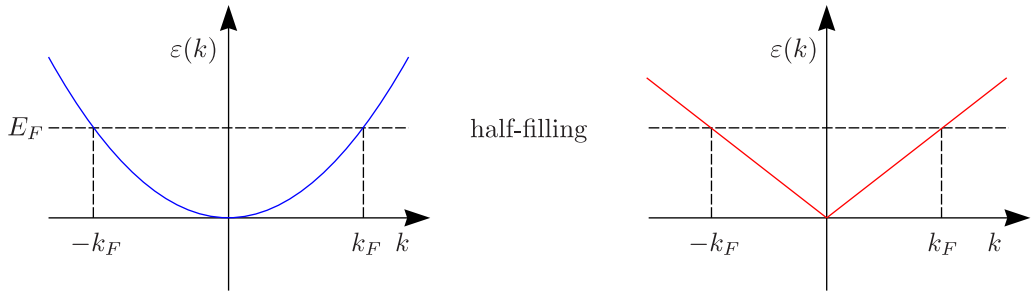
$$\boxed{\Delta = 2\omega_D \exp\left(-\frac{1}{|\lambda|\nu}\right), \Delta(T=0) = \frac{\pi}{\gamma} T_C\,.} \tag{6.63}$$

Electrons have interaction with the lattice even at zero temperature, so the phonons are not real but virtual.

Chapter 7

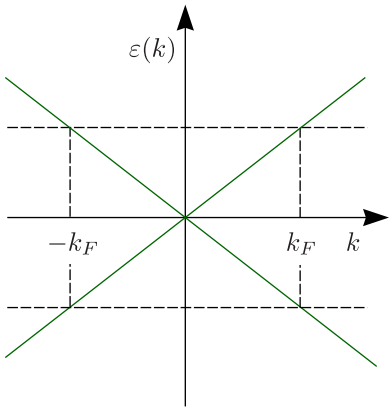
Interacting Fermions in a one-dimensional wire

In one dimension the dispersion relation of particles can considered to be relatively simple, namely quadratic.



particle spectrum linearized "Tomonaga model"

We will consider different types of scattering processes. They can be classified, whether they happen on the left-hand side or the right-hand side. If the energy exchange is small, the process will take place near the Fermi surface. We will linearize the dispersion relation near the vicinity of the Fermi surface. This approximation is called the linearized Tomonaga model. One can also introduce a cone:



If particles sit on the right-hand site all the time, they will be called right movers. Right movers and left movers obey different quantum numbers. This model is called the **Luttinger model**. For a parabolic dispersion relation it holds that

$$v_k = \frac{\partial \varepsilon}{\partial k} = \frac{p}{m} \,. \tag{7.1}$$

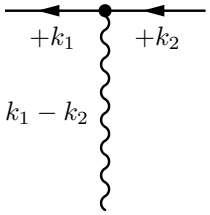
For the linearized version

$$\xi_k = \frac{k^2}{2m} - \mu \mapsto \begin{cases} (k - k_F) v_F \\ (-k - f_F) v_F \end{cases} \,, \tag{7.2}$$

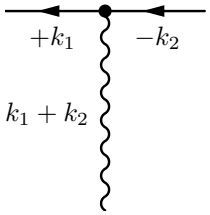
the velocity is independent of k: $v_k = v_F$. That will provide us an analytic solution for the many-body problem. The kinetic term in the Luttinger liquid looks like

$$H_0 = v_F \sum_k \left[(k - k_F) a^\dagger_{+k} a_{+k} + (-k - k_F) a^\dagger_{-k} a_{-k} \right] \,, \tag{7.3}$$

where "+" stands for the right-movers and "-" for the left-movers. What scattering processes are possible in terms of vertices?



These types of scattering processes involve an interaction $V(k_1 - k_2) \approx V(0)$, since the momentum change shall be small. They conserve the left and right quantum numbers and are therefore denoted as (+,+), (-,-). Another process to consider is that for left-movers, which turn into right-movers:



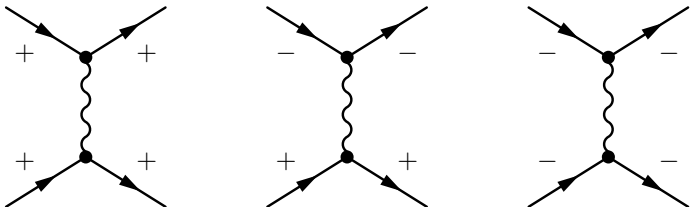
Since the particle has been scattered across the Fermi surface we will use $V(k_1 - k_2) \approx V(2k_F)$. These processes are denoted by (+,-), (-,+). Our model will not take these processes into account. Therefore, we will write

$$V(k_1 - k_2) \approx V(0) \approx g \qquad (+,+),\ (-,-)\,, \tag{7.4}$$

and

$$V(k_1 - k_2) \approx V(2k_F) \mapsto 0 \qquad (+,-),\ (-,+)\,. \tag{7.5}$$

Only:



$$H_{\text{int}} = \frac{g}{2L} \sum_q \sum_{\alpha=\pm} \left[\varrho_\alpha(q)\varrho_{-\alpha}(-q) + \varrho_\alpha(q)\varrho_\alpha(-q)\right]\,. \tag{7.6}$$

One could also consider a model with different coupling constants g_2 and g_4 for the different scattering processes. But here, we will set $g_2 = g_4 = g$. $\varrho_\alpha(q)$ are the density operators

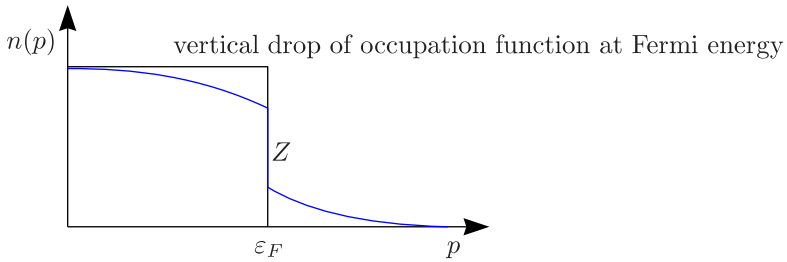
$$\varrho_\alpha(q) = \sum_k a^\dagger_{\alpha,k+q} a_{\alpha,k}\,. \tag{7.7}$$

The **Luttinger model (without spin)** is characterized by the sum $H_0 + H_{\text{int}}$. The goal is to do perturbation theory in H_{int} to get the self-energy Σ. Reminder:

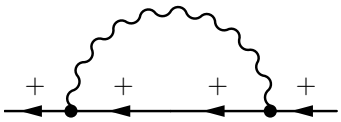
$$G(\varepsilon, p) \simeq \frac{Z}{\varepsilon - \xi_p + \frac{\mathrm{i}}{2}\Gamma(\varepsilon)\text{sign}(\varepsilon)}\,. \tag{7.8}$$

The residue Z had an important meaning. It could be calculated by

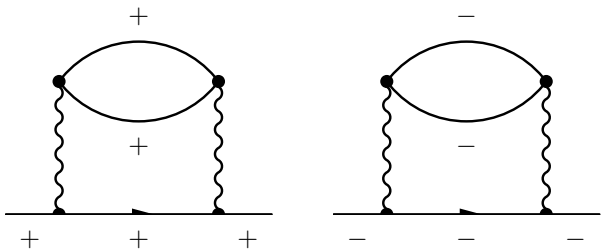
$$Z = \left.\frac{1}{1 - \frac{\partial}{\partial\varepsilon}\text{Re}(\Sigma(\varepsilon, p))}\right|_{\substack{p=p_F \\ \varepsilon=\varepsilon_F}}\,. \tag{7.9}$$

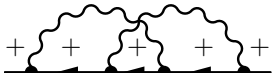


The drop has an infinite slope and this will dominate all quantities, which are calculated from the occupation function $n(p)$. Doing perturbation theory:

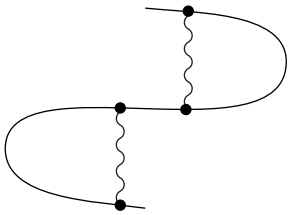


First order just shifts the chemical potential. So we will consider second order corrections to $\Sigma_+(\varepsilon, p)$. There are following contributions:





We will use a trick, with which we will only have to calculate one of the three diagrams. The sum of diagram (a) and (c) will vanish.



Hence, diagram (a) and (c) look the same, but the first one comes with an additional minus sign because of the fermionic loop and therefore the sum of (a) and (c) vanishes. Remark: Including spin it holds that (a) $= -2$(c). So, the cancelation only takes place in a model without spin. Now to the calculation of the remaining diagram:

$$\Sigma_+(\varepsilon, p) = \mathrm{i}^2 g^2 \int \frac{\mathrm{d}q\,\mathrm{d}\omega}{(2\pi)^2}\, \mathrm{i}\Pi_-(\omega, q) G_+^{(0)}(\varepsilon + \omega, p + q)\,, \tag{7.10}$$

with

$$G_\pm(\varepsilon, p) = \frac{1}{\varepsilon \mp v_F k + \mathrm{i}0\mathrm{sign}(\varepsilon)}\,, \tag{7.11}$$

and

$$\Pi_-(\omega, q) = \mathrm{i} \int \frac{\mathrm{d}\varepsilon'\,\mathrm{d}p'}{(2\pi)^2} G_-^{(0)}\left(\varepsilon' + \frac{\omega}{2}, p' + \frac{q}{2}\right) G_-^{(0)}\left(\varepsilon' - \frac{\omega}{2}, p' - \frac{q}{2}\right)\,. \tag{7.12}$$

A contour integration gives us

$$\Pi_-(\omega, q) = \frac{1}{2\pi} \frac{q}{v_F q + \omega + \mathrm{i}0\mathrm{sign}(\omega)}\,. \tag{7.13}$$

Hence, there exists a density wave of electrons which move like ordinary phonons in a crystal. Plugging (7.13) into the integral for Σ_+ yields

$$\mathrm{Re}(\Sigma_+(\varepsilon, p)) = \frac{g^2}{(2\pi)^2} \frac{1}{2v_F} (v_F p - \varepsilon) \int_0 \mathrm{d}q \left[\frac{1}{2v_F q + \varepsilon - v_F p} + \frac{1}{2v_F q - \varepsilon - v_F p}\right]\,. \tag{7.14}$$

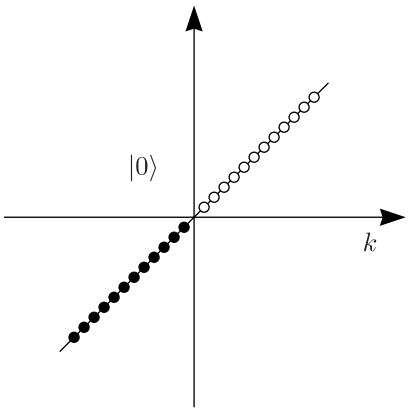
We need to introduce a UV cut-off $q_{\max}$, which leads us to the new energy scale $\Lambda = v_F q_{\max}$. The final answer is given by

$$\boxed{\mathrm{Re}(\Sigma_+(\varepsilon,p)) = -\frac{g^2}{(4\pi v_F)^2}(\varepsilon - v_F p)\ln\left(\frac{4\Lambda^2}{\varepsilon^2 - v_F^2 p^2}\right).} \tag{7.15}$$

We are coming to the calculation of Z:

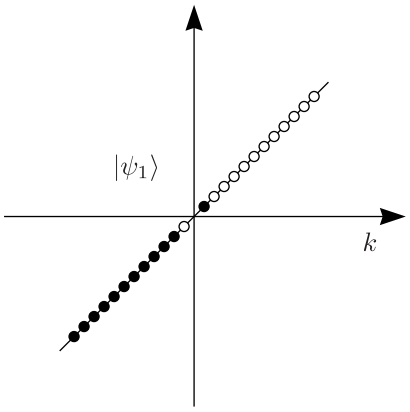
$$Z = \left.\frac{1}{1 - \frac{\partial}{\partial\varepsilon}\mathrm{Re}(\Sigma(\varepsilon,p))}\right|_{\substack{p=p_F\\ \varepsilon=\varepsilon_F}} = \frac{1}{1 + \frac{q^2}{(4\pi v_F)^2 \ln\left(\frac{\Lambda^2}{0}\right)}} = \boxed{0\,.} \tag{7.16}$$

This indicates that a Fermi liquid is not a good ground state. We need to go **from fermions to bosons**. Consider a fermionic chain with right movers.

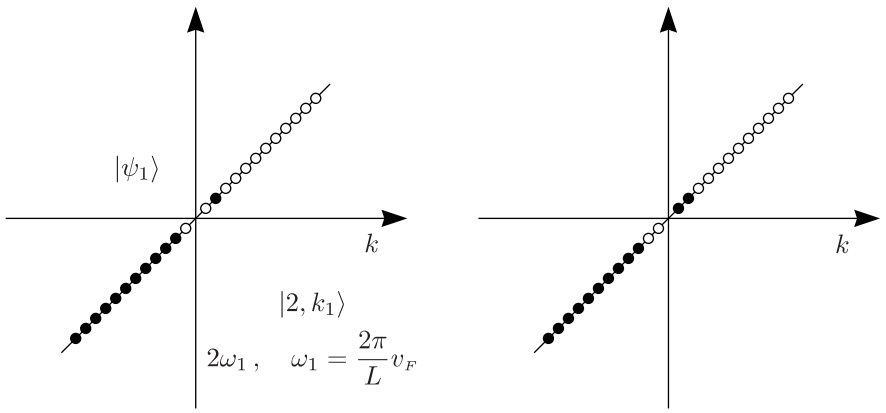


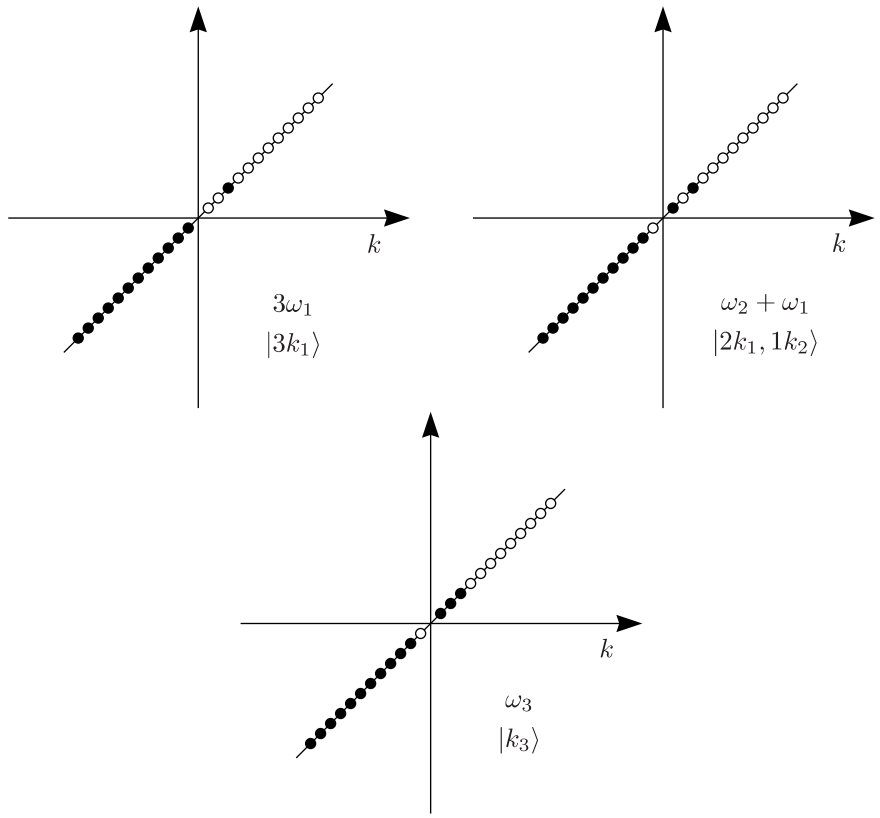
$$k_j = \frac{2\pi}{L} j\,, \quad \varepsilon_j = v_F k_j\,. \tag{7.17}$$

Excited state:



We could think of this state with one bosonic state $|1, k_1\rangle$.





We construct the Hilbert space of fermions by using bosons. Consider a superposition of operators the create the above states:

$$\widehat{\varrho}_q = \sum_k a^\dagger_{k+q} a_k \,. \tag{7.18}$$

It creates a boson with index $q = q_{(1)} - qL$, where L is the number of sites in the chain. The goal is to show that $\widehat{\varrho}_q$ corresponds to a bosonic operator. Write the Hamiltonian H_0 in terms of $\widehat{\varrho}_q$.

$$[\widehat{\varrho}_\alpha(q), \widehat{\varrho}_{\alpha'}(-q')] = \left[\sum_p \widehat{a}^\dagger_{\alpha,p+q}\widehat{a}_{\alpha,p}, \sum_{p'} \widehat{a}^\dagger_{\alpha',p'-q'}, \widehat{a}_{\alpha',p'}\right] = \delta_{\alpha\alpha'}\sum_p (\widehat{n}_{\alpha,p+q} - \widehat{n}_{\alpha,p}) \;, \quad \widehat{n}_{\alpha,p} = \widehat{a}^\dagger_{\alpha,p}\widehat{a}_{\alpha,p} =$$

$$= \delta_{\alpha\alpha'}(\text{number of particles mismatch}) = -\delta_{\alpha\alpha'}\sum_{p=p_0}^{q} \widehat{n}_{\alpha,p+q} = -\delta_{\alpha\alpha'}\frac{qL}{2\pi} \,. \tag{7.19}$$

Hence, we can argue that

$$\boxed{[\widehat{\varrho}_\alpha(q), \widehat{\varrho}_{\alpha'}(-q')] = \delta_{\alpha\alpha'}\delta_{qq'}\frac{(-\alpha)qL}{2\pi} \,.} \tag{7.20}$$

We will set $\alpha = +$ and obtain

$$\widehat{\varrho}_+(q) = \widehat{b}^\dagger_{+,q}\left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \,, \tag{7.21}$$

$$\widehat{\varrho}_+(-q) = \widehat{b}_{+,q}\left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \,, \tag{7.22}$$

for $q > 0$ and

$$\widehat{\varrho}_-(-q) = \widehat{b}^\dagger_{-,-q}\left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \,, \tag{7.23}$$

$$\widehat{\varrho}_-(q) = \widehat{b}_{-,-q}\left(\frac{qL}{2\pi}\right)^{\frac{1}{2}} \,, \tag{7.24}$$

for $q > 0$.

$$[\widehat{b}^\dagger_{\alpha,q}, \widehat{b}_{\alpha',q'}] = \delta_{\alpha\alpha'}\delta_{qq'} \,. \tag{7.25}$$

We will calculate

$$[\widehat{H}_0, \widehat{\varrho}_\alpha(q)] = \alpha v_F q \widehat{\varrho}_\alpha(q) \,. \tag{7.26}$$

In order to calculate the dynamics of the operators $\widehat{\varrho}$ the way of writing

$$\boxed{\widehat{H}_0 = \frac{\pi v_F}{L} \sum_{\alpha,q} \widehat{\varrho}_\alpha(q)\widehat{\varrho}_\alpha(-q) \,,} \tag{7.27}$$

gives the same dynamics as writing $\widehat{H}_0$ with $\widehat{a}^\dagger$ and $\widehat{a}$. Replace $\widehat{\varrho}$ by $\widehat{b}$ and $\widehat{b}^\dagger$ and solve $\widehat{H}_0 + \widehat{H}_{\text{int}}$ by Boguliubov transformation, which leads us to $\widehat{b}$ and $\widehat{b}^\dagger$:

$$\widehat{H} = \sum_{q>0} q \left[\left(v_F + \frac{g}{2\pi} \right)^2 - \left(\frac{g}{2\pi} \right)^2 \right]^{\frac{1}{2}} (\widetilde{b}^\dagger_{+,q}\widetilde{b}_{+,q} + \widetilde{b}_{-,-q}\widehat{b}_{-,-q}) \,, \tag{7.28}$$

with the dispersion relation $\omega = u|q|$ (look like acoustic phonons) and the velocity

$$u = \sqrt{\left(v_F + \frac{g}{2\pi} \right)^2 - \left(\frac{g}{2\pi} \right)^2} \,. \tag{7.29}$$

By repulsive interaction the particles will move faster.

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2.) Landau, Lifshitz: " Statistical Physics Part II" (IX)

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6.) Schrieffer: " Theory of superconductivity"

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8.) Altland, Simons: " Condensed Matter Field Theory"

Structure

0.) Introduction

1.) Green functions for non-interacting particles

2.) Many-body Green functions for $T = 0$

3.) Diagrammatrics for Fermi gas with weak interaction (Fermi liquids)

4.) Diagram techniques for $T \neq 0$ (Matsubara)

5.) Instabilities of a Fermi gas (Cooper-instability, superconductivity), Diagrammatrics for superconductive systems

6.) Interacting fermions in 1D, Luttinger liquid, Bosonization