Quantum Field Theory
for
Mesoscopic Transport

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Abstract

Quantum mechanics has been extremely useful for the description of material properties. The rapid development in control and manipulation of coherent quantum systems in recent years allows for the study and utilization of coherent quantum phenomena as well as the exploration of quantum mechanical concepts in realistic many-body setups. In such devices there exists a subtle interplay between a plethora of effects such as, disorder, interactions, and out-of-equilibrium noise that compete and limit the regimes in which coherence survives. To describe the transport properties of such devices one requires more suitable tools that can take into account the interplay between these effects. In the proseminar, we shall review theoretical tools (both analytic and numerical) that have been developed to address such transport phenomena. These tools are actively used in contemporary research , are deeply linked to questions in quantum information theory, and are also an integral tool in the study of topological phenomena. We shall apply these methods to study realistic models.

In this proseminar, field theoretical methods for the description of many-body transport phenomena will be discussed.

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Chapter 1

Introduction

An overview over some basic methods

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This chapter is an introduction to the basic concepts and methods we will use later. We start with the general Hamiltonian of a solid and make some assumptions to simplify it. We introduce Green's functions to solve inhomogeneous differential equations such as the single particle Schrödinger equation. We introduce Bloch's theorem to deal with a single electron under a periodic potential. We also introduce the Fermi liquid theory to deal with interacting electrons in a metal.

1.1 The Hamiltonian of a Solid

We consider a solid as a lattice of ions with electrons between the ions as depicted in Fig. 1.1. In general, such a system can be described by a Hamiltonian of the structure

$$H = H_{\text{ion}} + H_{\text{el}} + H_{\text{el-ion}}, \tag{1.1}$$

where H_{ion} describes the kinetics and the interaction of only the ions, H_{el} describes the kinetics and the interaction of only the electrons and $H_{\text{el-ion}}$ describes the interaction between the

[1] supervised by Mark H. Fischer

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Figure 1.1 Solid consisting of ions (gray) and electrons (blue). [1]

ions and the electrons. We can write each of the constituents as follows:

$$
\begin{aligned}
H_{\text{ion}} &= \sum_{i=1}^{N_{\text{ion}}} \frac{\mathbf{P}_i^2}{2M_i} + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_{\text{ion}}} V(\mathbf{R}_i - \mathbf{R}_j) \\
H_{\text{el}} &= \sum_{l=1}^{N_{\text{el}}} \frac{\mathbf{p}_l^2}{2m} + \frac{1}{2} \sum_{\substack{k,l=1 \\ k \neq l}}^{N_{\text{el}}} \frac{e^2}{4\pi\varepsilon_0 |\mathbf{r}_l - \mathbf{r}_k|} \\
H_{\text{el-ion}} &= \sum_{l=1}^{N_{\text{el}}} \sum_{i=1}^{N_{\text{ion}}} v(\mathbf{r}_l - \mathbf{R}_i),
\end{aligned}
\tag{1.2}
$$

where

- $\mathbf{P}_i$, M_i and $\mathbf{R}_i$ are momentum, mass and position respectively of the i-th ion,
- $\mathbf{p}_l$ and $\mathbf{r}_l$ are momentum and position respectively of the l-th electron and m is the electron mass,
- V and v are two potentials and
- N_{ion} and N_{el} are the total number of ions and electrons respectively.

We will now make some assumptions to simplify the Hamiltonian for some particular problems.

1.1.1 Born-Oppenheimer approximation

The Born-Oppenheimer approximation is the assumption that the nuclear kinetic energy can be neglected and therefore, the nuclear positions enter as parameters in the remaining Hamiltonian [2]. It is legitimate because heavy and light particles change their directions of motion on very different time scales such that the equations of motion of the fast, light particles can be solved without considering the motion of the slow, heavy ones. This affects the ionic and the interaction part of the Hamiltonian as follows:

$$
H_{\text{ion}} + H_{\text{el-ion}} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_{\text{ion}}} V(\mathbf{R}_i^0 - \mathbf{R}_j^0) + \sum_{l=1}^{N_{\text{el}}} \sum_{i=1}^{N_{\text{ion}}} v(\mathbf{r}_l - \mathbf{R}_i^0). \tag{1.3}
$$

Note that the zero superscripts denote the constant position and the kinetic term of the ion part can be neglected due to the assumption.

We can furthermore combine the two potential terms to one single-particle potential $V(\mathbf{r}_l)$ as a function of only the electron positions:

$$\sum_{l=1}^{N_{\text{el}}} V(\mathbf{r}_l) = \underbrace{\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N_{\text{ion}}} V(\mathbf{R}_i^0 - \mathbf{R}_j^0)}_{\equiv\text{const.}} + \sum_{l=1}^{N_{\text{el}}}\sum_{i=1}^{N_{\text{ion}}} v(\mathbf{r}_l - \mathbf{R}_i^0). \tag{1.4}$$

We do that to obtain the following simple form of the Hamiltonian:

$$H = \sum_{l=1}^{N_{\text{el}}}\left[\frac{\mathbf{p}_l^2}{2m} + V(\mathbf{r}_l)\right] + \frac{1}{2}\sum_{\substack{k,l=1\\ k\neq l}}^{N_{\text{el}}} \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_l - \mathbf{r}_k|}. \tag{1.5}$$

First, we will neglect the electron-electron interaction and only consider the first term for a single electron and without any further assumptions on the potential. We will then take another step towards the description of solids by the assumption of the potential to be perfectly periodic, as expected for an electron scattering in a crystal, for instance a metal or a semiconductor. Finally, we also include the electron-electron interaction and give an overview on Fermi-Liquid theory where we use some simple assumptions to get rid of the potential.

1.2 Scattering of a free electron

As already mentioned in the introduction, we will only consider the first term of the Hamiltonian (1.5) for a single electron. Thus, we have a Hamiltonian of the form

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \tag{1.6}$$

Denoting the eigenstates of this Hamiltonian by $\psi_{\mathbf{k}}$ and the corresponding eigenenergies by E_k, we can write the time-independent Schrödinger equation of our problem as

$$\left[-\frac{\hbar^2}{2m}\nabla_x^2 + V(\mathbf{x})\right]\psi_{\mathbf{k}}(\mathbf{x}) = E_k\psi_{\mathbf{k}}(\mathbf{x}). \tag{1.7}$$

In order to solve this differential equation, we want to introduce the concept of Green's functions which we will also use many times in the upcoming chapters.

1.2.1 Green's functions

Green's functions help us to solve inhomogeneous differential equations. We consider a very general differential equation

$$\hat{L}_x u(x) = f(x), \tag{1.8}$$

where $\hat{L}_x$ is a differential operator acting on x, $u(x)$ is the unknown solution and $f(x)$ is the inhomogeneous part. Instead of solving this equation directly, we can define a Green's function $G(x)$ for the operator $\hat{L}_x$. Such a Green's function is defined by the differential equation

$$\hat{L}_x G(x) = \delta(x), \tag{1.9}$$

where $\delta(x)$ is the Dirac delta distribution. We can write a particular solution of our original Eq. (1.8) in the form

$$u(x) = \int \mathrm{d}y\, G(x-y) f(y). \tag{1.10}$$

This can easily be seen when we apply the operator $\hat{L}_x$ on this solution:

$$\begin{aligned} \hat{L}_x u(x) &= \int \mathrm{d}y\, \hat{L} G(x-y) f(y) \\ &= \int \mathrm{d}y\, \delta(x-y) f(y) \\ &= f(x). \end{aligned} \tag{1.11}$$

At first sight, it is not clear why this is useful since we still have to solve the differential equation (1.9). To see what are the benefits of this method, we consider an example from electrostatics.

Example: Poisson's equation

In electrostatics, an electric potential $\varphi(\mathbf{x})$ satisfies Poisson's equation

$$\nabla_x^2 \varphi(\mathbf{x}) = -\frac{1}{\varepsilon_0} \varrho(\mathbf{x}), \tag{1.12}$$

where $\varrho(\mathbf{x})$ is the charge distribution. We can identify ∇_x^2 as the differential operator, $\varphi(\mathbf{x})$ as the unknown solution and $-\frac{1}{\varepsilon_0}\varrho(\mathbf{x})$ as the inhomogeneous part of the differential equation. Thus we define the corresponding Green's function by

$$\nabla_x^2 G(\mathbf{x}) = \delta^3(\mathbf{x}). \tag{1.13}$$

We now want to solve this defining equation explicitly for $G(\mathbf{x})$. To do so, we apply a Fourier transform on both sides of the equation

$$\begin{aligned} \int \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \nabla_x^2 G(\mathbf{x}) &= \int \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \delta^3(\mathbf{x}) \\ -k^2 \tilde{G}(\mathbf{k}) &= 1 \\ \tilde{G}(\mathbf{k}) &= -\frac{1}{k^2}. \end{aligned} \tag{1.14}$$

Here, $\tilde{G}(\mathbf{k})$ is the Fourier transform of $G(\mathbf{x})$. We can apply the inverse Fourier transform to obtain the Green's function in position space,

$$\begin{aligned} G(\mathbf{x}) &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tilde{G}(\mathbf{k}) \\ &= -\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{k^2} \\ &= -\frac{1}{4\pi|\mathbf{x}|}. \end{aligned} \tag{1.15}$$

We can plug this in (1.10) and obtain the familiar expression for the electric potential

$$\varphi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \mathrm{d}^3\mathbf{y}\, \frac{\varrho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}. \tag{1.16}$$

1.2.2 Lippmann-Schwinger equation

We now want to apply the introduced techniques to a more sophisticated example. Consider the time-independent Schrödinger equation of a state ψ_E with Hamiltonian H and eigenenergy E:

$$H\psi_E = E\psi_E. \tag{1.17}$$

For a system of incoming particles described by the Hamiltonian H_0 scattering at a potential $V(\mathbf{x})$, we can write our Hamiltonian as

$$H(\mathbf{x}) = H_0(\mathbf{x}) + V(\mathbf{x}). \tag{1.18}$$

We assume that the potential is weak, i.e. $|\mathbf{x}|V(\mathbf{x}) \to 0$, and therefore only a little perturbation to the incoming waves. With this assumption, we can expect the eigenenergy of H_0 to be the same as for the whole system. Therefore, the eigenstates $\psi_E^{(0)}$ of the incoming waves can be described by the time-independent Schrödinger equation

$$H_0\psi_E^{(0)} = E\psi_E^{(0)}. \tag{1.19}$$

We now insert the Hamiltonian (1.18) into Eq. (1.17) and can write after rearranging

$$[E - H_0(\mathbf{x})]\psi_E(\mathbf{x}) = V(\mathbf{x})\psi_E(\mathbf{x}). \tag{1.20}$$

We can interpret this as a differential equation with the square bracket being the differential operator, $\psi_E(\mathbf{x})$ being the unknown function and $V(\mathbf{x})\psi_E(\mathbf{x})$ being the inhomogeneous part. Note that the inhomogeneous part also contains the unknown function. We will see later how we can solve this problem. We can define the Green's function of $[E - H_0(\mathbf{x})]$ by the equation

$$[E - H_0(\mathbf{x})]G(\mathbf{x}) = \delta^3(\mathbf{x}). \tag{1.21}$$

The formal solution is now a superposition of the solution of the homogeneous problem (1.19) and a particular solution of (1.20), where the latter is again given by an integral containing the Green's function:

$$\psi_E(\mathbf{x}) = \psi_E^{(0)}(\mathbf{x}) + \int \mathrm{d}^3\mathbf{y}\, G(\mathbf{x} - \mathbf{y})V(\mathbf{y})\psi_E(\mathbf{y}). \tag{1.22}$$

This equation is known as the Lippmann-Schwinger equation.

Note that we didn't specify our Hamiltonian $H_0(\mathbf{x})$ yet. In the next subsection, we will do this and also find an explicit expression for the Green's function.

1.2.3 Scattering of an incoming plane wave

We now go back to where we started and consider the Hamiltonian (1.6) of an incoming free particle scattering at a potential $V(\mathbf{x})$. The Hamiltonian of the incoming particle then has the form

$$H_0(\mathbf{x}) = \frac{\mathbf{p}^2}{2m} = \frac{-\hbar^2}{2m}\nabla_x^2. \tag{1.23}$$

If we only have an incident particle, the eigenstates and eigenenergies can be written as

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \quad E_k = \frac{\hbar^2 k^2}{2m} \quad \text{where} \quad k = |\mathbf{k}|. \tag{1.24}$$

We plug (1.23) into the differential equation for the Green's function (1.21) and obtain

$$\left[E_k + \frac{\hbar^2}{2m}\nabla_x^2\right]G(\mathbf{x}) = \delta^3(\mathbf{x}). \tag{1.25}$$

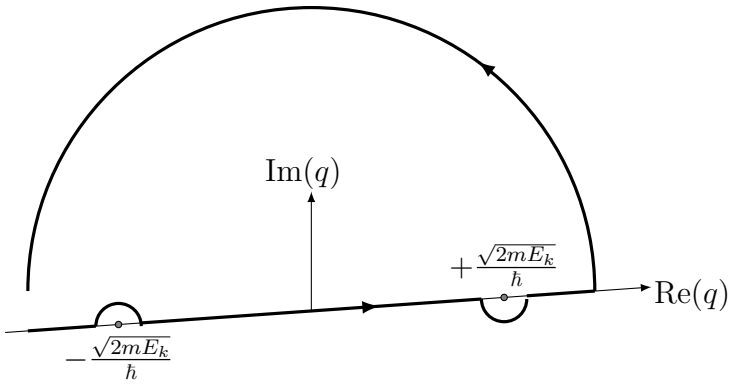

Figure 1.2 Contour of integration of an integral with poles at $q = \pm\frac{\sqrt{2mE_k}}{\hbar}$ where the positive pole is included.

As in the case of the Poisson's equation (1.13), we apply a Fourier transform to this equation and find an explicit expression for the Fourier transform of the Green's function:

$$\tilde{G}(\mathbf{q}, E_k) = \frac{1}{E_k - \varepsilon_q}, \quad \varepsilon_q = \frac{\hbar^2 q^2}{2m}. \tag{1.26}$$

Transforming back to position space and changing to spherical coordinates, we have

$$\begin{aligned} G(\mathbf{x}, E_k) &= \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}}}{E_k - \varepsilon_q} \\ &= -\frac{m}{2\pi^2\hbar^2 \mathrm{i}|\mathbf{x}|} \int_{-\infty}^{\infty} q\,\mathrm{d}q\, \frac{\mathrm{e}^{\mathrm{i}q|\mathbf{x}|}}{\frac{2mE_k}{\hbar^2} - q^2}. \end{aligned} \tag{1.27}$$

The remaining integral can be considered as a line integral in the complex plane with poles at $q = \pm\frac{\sqrt{2mE_k}}{\hbar}$. Since these poles are on the real axis, we cannot just choose our contour along the real axis, we must also go around the poles and either include or exclude them in order to apply the residue theorem. The physical requirements for our solution (i.e. the scattered wave being an outgoing wave) tell us to include the positive pole but to exclude the negative one as depicted in Fig. 1.2. We close the contour on the upper half-plane since the integral along the arc vanishes for $|\mathbf{x}| > 0$ and $q \to \infty$. Applying the residue theorem, we obtain

$$G(\mathbf{x}, E_k) = -\frac{m}{2\pi\hbar^2} \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|}. \tag{1.28}$$

We can plug Eq. (1.24) and (1.28) back into the Lippman-Schwinger equation (1.22) and find

$$\psi_{\mathbf{k}}(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} - \frac{m}{2\pi\hbar^2} \int \mathrm{d}^3\mathbf{y}\, \frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} V(\mathbf{y})\psi_{\mathbf{k}}(\mathbf{y}). \tag{1.29}$$

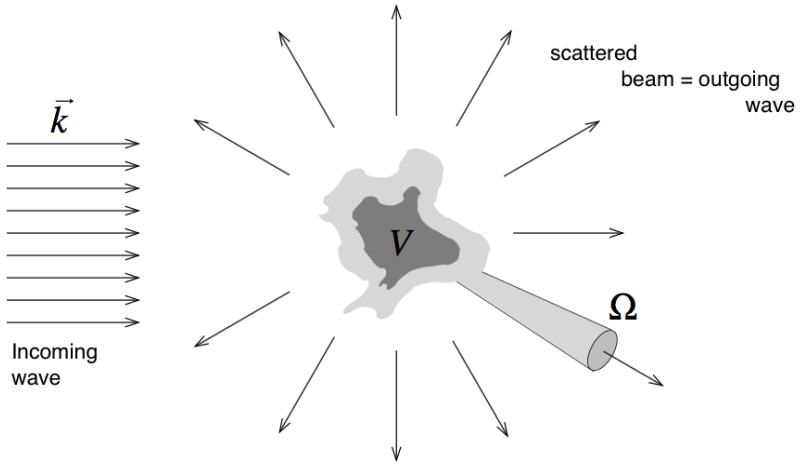

Figure 1.3 Geometry of an incoming plane wave scattering at a potential and propagating as a spherical wave. [3]

1.2.4 Scattering amplitude and cross-section

We now want to interpret the Lippmann-Schwinger equation (1.29) at large distances. We assume the scattered wave to propagate as a spherical wave (see Fig. 1.3 and therefore expect the following form at large distances $|\mathbf{x}| \to \infty$:

$$\psi_{\mathbf{k}}(\mathbf{x}) \sim \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} + f_k(\Omega)\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|}, \tag{1.30}$$

where $f_k(\Omega)$ is the scattering amplitude. We can see that the first term already matches (1.29), but the second does not yet, so we also expand Eq. (1.29) for $|\mathbf{x}| \to \infty$:

$$\psi_{\mathbf{k}}(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} V(\mathbf{y})\psi_{\mathbf{k}}(\mathbf{y})\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|}, \tag{1.31}$$

where $\mathbf{k}' = k\mathbf{e}_{|\mathbf{x}|}$ and identify the scattering amplitude

$$f_k(\Omega) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} V(\mathbf{y})\psi_{\mathbf{k}}(\mathbf{y}). \tag{1.32}$$

We now want to connect this amplitude to the cross-section. The differential cross-section is defined by

$$\begin{aligned} \mathrm{d}\sigma &\equiv \frac{\#\text{ of scattered particles in } \mathrm{d}\Omega \text{ per time}}{\#\text{ of incoming particles per time and area}} \\ &= \frac{j_{\mathrm{scat}} r^2\, \mathrm{d}\Omega}{j_{\mathrm{in}}}, \end{aligned} \tag{1.33}$$

where j_{in} and j_{scat} are the current densities of the incoming and the scattered wave, respectively,

$$\mathbf{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{1.34}$$

With this definition, we find

$$\begin{aligned} j_{\text{in}} &= \frac{\hbar k}{m}, \\ j_{\text{scat}} &= \frac{\hbar k}{m}\frac{1}{r^2}|f_k(\Omega)|^2 + \mathcal{O}\big(r^{-3}\big), \end{aligned} \tag{1.35}$$

and can plug this into Eq. (1.33)

$$\mathrm{d}\sigma = |f_k(\Omega)|^2\,\mathrm{d}\Omega\,. \tag{1.36}$$

The total cross-section is obtained by integration

$$\sigma = \int \mathrm{d}\Omega\,|f_k(\Omega)|^2. \tag{1.37}$$

1.2.5 Born approximation

The Lippmann-Schwinger equation (1.31) still depends on $\psi_{\mathbf{k}}$, i.e. we have an infinite series

$$\psi_{\mathbf{k}}(\mathbf{x}) = \psi^{(0)}_{\mathbf{k}}(\mathbf{x}) + \sum_{n=1}^{\infty}\delta\psi^{(n)}_{\mathbf{k}}(\mathbf{x}) \tag{1.38}$$

with

$$\begin{aligned} \psi^{(0)}_{\mathbf{k}}(\mathbf{x}) &= \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \delta\psi^{(0)}_{\mathbf{k}}(\mathbf{x}), \\ \delta\psi^{(1)}_{\mathbf{k}}(\mathbf{x}) &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{y}}V(\mathbf{y})\delta\psi^{(0)}_{\mathbf{k}}(\mathbf{y})\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|}, \\ &\vdots \\ \delta\psi^{(n)}_{\mathbf{k}}(\mathbf{x}) &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{y}}V(\mathbf{y})\delta\psi^{(n-1)}_{\mathbf{k}}(\mathbf{y})\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|}. \end{aligned}$$

Stopping the expansion at $n = N$ is called the N-th Born approximation

$$\psi^{(N)}_{\mathbf{k}}(\mathbf{x}) = \sum_{n=0}^{N}\delta\psi^{(n)}_{\mathbf{k}}(\mathbf{x}). \tag{1.39}$$

For high particle energies and weak scattering potentials, the first Born approximation is a good approximation. We can write

$$\psi_{\mathbf{k}}^{(1)}(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} - \frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\, V(\mathbf{y})\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}}\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{x}|}}{|\mathbf{x}|} \tag{1.40}$$

and find the scattering amplitude

$$f_k^{(1)}(\Omega) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3\mathbf{y}\, V(\mathbf{y})\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}}. \tag{1.41}$$

The latter is also called the Born amplitude and is basically a Fourier transform of the scattering potential. The integral is a matrix element of the scattering potential, thus

$$\langle\mathbf{k}'|\, V\,|\mathbf{k}\rangle = \int \mathrm{d}^3\mathbf{y}\, V(\mathbf{y})\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}}. \tag{1.42}$$

Example: Coulomb potential

We now want to derive the differential cross-section of a Coulomb potential explicitly. We define the momentum transfer $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and write its magnitude

$$q = |\mathbf{k} - \mathbf{k}'| = 2k\sin\left(\frac{\theta}{2}\right), \tag{1.43}$$

where $\theta = \measuredangle(\mathbf{k}, \mathbf{k}')$ is the angle between the two vectors $\mathbf{k}$ and $\mathbf{k}'$. For a central potential $V(\mathbf{x}) = V(|\mathbf{x}|)$, we can rewrite the matrix element

$$\begin{aligned}\langle\mathbf{k}'|\, V\,|\mathbf{k}\rangle &= \int_0^\infty \mathrm{d}r\, r^2 \int_0^{2\pi}\mathrm{d}\varphi \int_{-1}^{1}\mathrm{d}(\cos\vartheta)\, V(r)\mathrm{e}^{\mathrm{i}qr\cos\vartheta} \\ &= \frac{4\pi}{q}\int_0^\infty \mathrm{d}r'\, r' V(r')\sin(qr').\end{aligned} \tag{1.44}$$

Plugging in the Coulomb potential

$$V(r) = \frac{Ze^2}{4\pi\varepsilon_0 r} = \frac{C}{r}, \tag{1.45}$$

we have

$$\begin{aligned}\int_0^\infty \mathrm{d}r'\, r' V(r')\sin(qr') &= C\int_0^\infty \mathrm{d}r'\sin(qr') \\ &= \frac{C}{q} = \frac{Ze^2}{4\pi\varepsilon_0 q}.\end{aligned} \tag{1.46}$$

We introduced a small parameter ϵ to regularize the integral.

The differential cross-section then is given by

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \left|f_k^{(1)}(\Omega)\right|^2 \\ &= \frac{m^2}{4\pi^2\hbar^4}|\langle \mathbf{k}'|\, V\, |\mathbf{k}\rangle|^2 \\ &= \left(\frac{m}{2\pi\hbar^2}\frac{4\pi}{q}\right)^2\left(\frac{Ze^2}{4\pi\varepsilon_0 q}\right)^2 \\ &= \frac{1}{16E^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2 \sin^{-4}\left(\frac{\theta}{2}\right),\end{aligned} \tag{1.47}$$

which is just Rutherford's formula.

1.3 Bloch theory

In the previous section we focussed on the scattering of a free electron at a potential that we interpreted as a small perturbation with respect to the Hamiltonian of a free electron. The so-called Born approximation has been introduced and discussed. In this Section, we want to take another step towards the description of solids, in particular metals, insulators and semiconductors. This step is to assume a periodic potential as a simplified model of a solid, while still disregarding the electron-electron interaction, lattice impurities and the electron-phonon-interaction. The solid is modeled as a rigid lattice of atoms which in turn gives rise to the periodic potential. Let our lattice be a so-called Bravais lattice, where at each point of the set

$$\mathrm{BL} := \left\{ \mathbf{R}_\mathbf{n} = \sum_{i=1}^{3} n_i \mathbf{a}_i \;\middle|\; \mathbf{n} \in \mathbb{Z}^3 \right\} \tag{1.48}$$

there is an atom with a potential V_{atom}. Here $(\mathbf{a}_i)_{i\in(1,2,3)}$ is a basis of $\mathbb{R}^3$ and let $(\mathbf{b}_i)_{i\in(1,2,3)}$ be its corresponding dual basis defined by $\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij}$. Adding up all the identical but shifted potentials of the atoms results in a total potential V which is periodic.

Due to the fact that we are not taking electron-electron-interactions into account, our Hamiltonian is effectively a single-particle Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}), \tag{1.49}$$

where here, however, the potential V is periodic with respect to the lattice. In formal language, the potential V has to be invariant with respect to the action of the space group

of the lattice. In particular, V is then invariant with respect to the action of the translation subgroup. Labeling the action of a translation $\mathbf{R_n}$ by $T_\mathbf{n} \in \mathrm{GL}(\{f\colon \mathbb{R}^3 \to \mathbb{C}\})$, we can formalize the above statement by

$$\forall \mathbf{n} \in \mathbb{Z}^3\colon\ (T_\mathbf{n} V)(\mathbf{r}) \overset{\text{def}}{=} V(\mathbf{r}+\mathbf{R_n}) \overset{!}{=} V(\mathbf{r})\,. \tag{1.50}$$

Before moving on, let us now try to apply the previously introduced first-order perturbation theory method to such a periodic potential. Clearly, this in the first place already doesn't sound like a very good approach (due to the non-compact support of V), but let us explicitly observe how it fails.

Suppose we are given an electron in a state which corresponds to a free electron of momentum $\hbar\mathbf{k}$. We might want to calculate the transition rate according to Fermi's Golden rule for such an electron when put into a periodic potential of the form $V(\mathbf{r}) = \sum_\mathbf{n} V_\text{atom}(\mathbf{r}-\mathbf{R_n})$. Doing so yields

$$\begin{aligned}
\Gamma_{\mathbf{k}\to\mathbf{k}'} &= \frac{2\pi\rho}{\hbar}\left|\left\langle \mathbf{k}'\middle|\sum_\mathbf{n} V_\text{atom}(\mathbf{r}-\mathbf{R_n})\middle|\mathbf{k}\right\rangle\right|^2 \\
&= \frac{2\pi\rho}{\hbar}\left|\sum_\mathbf{n} \underbrace{\int \mathrm{d}^3\mathbf{r}\; e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}-\mathbf{R_n})} V_\text{atom}(\mathbf{r}-\mathbf{R_n})}_{=:\, f(\mathbf{k}-\mathbf{k}')}\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R_n}}\right|^2 \\
&= \frac{2\pi\rho}{\hbar}\,|f(\mathbf{k}-\mathbf{k}')|^2 \sum_{\mathbf{n},\mathbf{m}} e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{R_n}-\mathbf{R_m})} \\
&= \frac{2\pi\rho}{\hbar}\,|f(\mathbf{k}-\mathbf{k}')|^2 \sum_\mathbf{n} \left[\delta\left(\mathbf{k}-\mathbf{k}'+\sum_{i=1}^3 n_i\mathbf{b}_i\right)\right]^2,
\end{aligned} \tag{1.51}$$

where ρ is the density of states at the energy of the free electron. We observe that for any $\mathbf{k}'$ that differs from $\mathbf{k}$ by an integer linear combination of the dual basis $(\mathbf{b}_i)_{i\in(1,2,3)}$ on $\mathbb{R}^3$ the transition rate diverges and we are left with a series of squares of delta distributions which is a hard to interpret result in this context. What we have to deduce, however, is that we cannot attribute a finite lifetime $\tau_\mathbf{k}$ to a state of momentum $\hbar\mathbf{k}$, due to the divergencies. Physically speaking, the state which corresponds to a free electron of momentum $\hbar\mathbf{k}$ is instantaneously decomposed by the periodic lattice in place. This can be understood as a mathematical manifestation of Bragg diffraction. Our assumption of the free-electron energy eigenstates being approximately held in place even when switching on the periodic potential turns out to be utterly wrong. Finite order perturbation theory is not working out here and we are left with no other option than to reconsider the given problem.

1.3.1 Bloch's theorem

As the perturbation theory approach failed, we might want to address the problem of explicitly finding the exact energy eigenstates of the Hamiltonian. While this is very ambitious, we would also be satisfied with finding far-reaching conclusions about the spectrum of the Hamiltonian and its eigenstates.

The standard idea would be to extract information about the spectrum $\sigma(H)$ and the eigenstates of H, by employing the symmetry-group of H that we are given, here, the space group of the lattice. It turns out that if we tried to approach the problem of the spatially indefinitely extended lattice, we would fail to draw valuable conclusions due to handling with infinite-dimensional non-separable topological vector spaces and possibly infinite-dimensional irreducible representations of the translation group on such.

Therefore, we substitute the problem by a simpler one. Instead of assuming a spatially indefinitely extended lattice, we will focus on a patch of lattice with periodic boundary conditions. Consider a patch of a lattice

$$\text{Cell} := \left\{ \sum_{i=1}^{3} \lambda_i \mathbf{a}_i \;\middle|\; \forall\, 1 \leq i \leq 3 \colon 0 \leq \lambda_i \leq N_i \right\} \tag{1.52}$$

with atoms at positions

$$\text{Lattice} := \left\{ \sum_{i=1}^{3} \left(n_i + \frac{1}{2} \right) \mathbf{a}_i \;\middle|\; \forall\, 1 \leq i \leq 3 \colon n_i \in \mathbb{Z}_{N_i} \right\}, \tag{1.53}$$

where $(\mathbf{a}_i)_{i\in(1,2,3)}$ is a basis of $\mathbb{R}^3$ as above and where $\mathbb{Z}_N = \{n \in \mathbb{Z} \mid 1 \leq n \leq N\}$ are the elements of the standard integer representation of the cyclic group of order N with respect to modular addition. Our initial separable Hilbert space would be the space of equivalence classes of almost everywhere equal square-integrable functions on our domain $\mathrm{L}^2(\text{Cell})$. With respect to our cell we will assume periodic boundary conditions, and therefore restrict our Hilbert space further. It is easy to see that this subspace $\mathcal{H} := \mathrm{L}^2(\text{Cell})_{\text{periodic}}$ is still a separable Hilbert space. In particular one can show that there exists a unique self-adjoint extension of our momentum operator that we are familiar with. We thus can write down our Hamiltonian as we wish as

$$H := \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}), \tag{1.54}$$

where we explicitly require the potential $V(\mathbf{r})$ to be periodic with respect to the lattice, i.e.

$$\begin{aligned} &\forall \mathbf{n} = (n_1, n_2, n_3) \in \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} : \\ (T_{\mathbf{n}} V)(\mathbf{r}) &\overset{\text{def}}{=} V\left(\mathbf{r} + \sum_{i=1}^{3} \left(n_i - N_i \left\lfloor \frac{\frac{\mathbf{r}\cdot\mathbf{a}_i}{\|\mathbf{a}_i\|} + n_i}{N_i} \right\rfloor \right) \mathbf{a}_i \right) \overset{!}{=} V(\mathbf{r}). \end{aligned} \tag{1.55}$$

Here we have already introduced the representation of the finite translation group on the space of Cell-periodic functions

$$T \colon \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} \to \mathrm{GL}\left(\{f \colon \mathrm{Cell} \to \mathbb{C} \mid f \text{ Cell-periodic}\}\right), \ \mathbf{n} \mapsto T_{\mathbf{n}}. \tag{1.56}$$

In other terms, $T_{\mathbf{n}=(n_1,n_2,n_3)}$ shifts a function by n_1 atoms in $-\mathbf{a}_1$-direction, n_2 atoms in $-\mathbf{a}_2$-direction and n_3 atoms in $-\mathbf{a}_3$-direction. Note that by our requirement for V, we have

$$\forall \mathbf{n} \in \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} \colon \ [H, T_{\mathbf{n}}] = 0. \tag{1.57}$$

What this tells us is that any eigenspace $\mathcal{H}_E$ of H to any eigenvalue E is an invariant subspace with respect to our translation group representation.

It can be shown that H has a pure point spectrum and to each eigenvalue E of H, the corresponding eigenspace $\mathcal{H}_E$ is finite-dimensional.[2]

Thus for any eigenvalue E of H, the restriction of our translation group representation T to the corresponding eigenspace $\mathcal{H}_E$ is then a finite-dimensional complex representation.

As the translation group of the patch of crystal with periodic boundary conditions is a finite group, we recall from the theory of finite groups that any finite-dimensional complex representation is completely reducible. Furthermore, recall that as the translation group is abelian, any finite-dimensional complex irreducible representation is one-dimensional. These two results enable us to decompose the finite-dimensional complex representation of T on $\mathcal{H}_E$ into a finite sum of one-dimensional complex irreducible representations. Translating this into a language in terms of bases, we realize that this tells us that we can find a basis $\psi_1, \ldots, \psi_{\dim \mathcal{H}_E}$ such that each basis vector spans a one-dimensional invariant subspace corresponding to a one-dimensional complex irreducible representation of the translation group

$$\forall\ 1 \leq l \leq \dim \mathcal{H}_E \colon \forall \mathbf{n} \in \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} \colon \exists \lambda_{\mathbf{n},l} \in \mathbb{C} \colon T_{\mathbf{n}} \psi_l = \lambda_{\mathbf{n},l} \psi_l. \tag{1.58}$$

Note that for each $1 \leq l \leq \dim \mathcal{H}_E$ $\lambda_{\mathbf{n},l}$ is a one-dimensional complex irreducible representation of the translation group. We can now either argue with the boundary conditions or alternatively with the concrete realization that the translation group in our case is just a

[2] It turns out that H has compact resolvent [6, Theorem XIII.76]. Further, note that a densely defined symmetric operator with compact resolvent has pure point spectrum with corresponding finite-dimensional eigenspaces [7, Theorem 1.7.16].

direct sum of three cyclic groups $\mathbb{Z}_{N_1} \oplus \mathbb{Z}_{N_2} \oplus \mathbb{Z}_{N_3}$, in order to arrive at the conclusion that our group generators $T_{(1,0,0)}$, $T_{(0,1,0)}$ and $T_{(0,0,1)}$ are of the form

$$\begin{gathered}\forall\ 1 \leq l \leq \dim \mathcal{H}_E \colon \exists m_{1,l} \in \mathbb{Z}_{N_1}, m_{2,l} \in \mathbb{Z}_{N_2}, m_{3,l} \in \mathbb{Z}_{N_3} \colon \\ \left[\lambda_{(1,0,0),l} = e^{i2\pi \frac{m_{1,l}}{N_1}} \wedge \lambda_{(0,1,0),l} = e^{i2\pi \frac{m_{2,l}}{N_2}} \wedge \lambda_{(0,0,1),l} = e^{i2\pi \frac{m_{3,l}}{N_3}}\right].\end{gathered} \tag{1.59}$$

Applying an arbitrary translation to one of the basis vectors ψ_l, we now see that we can write

$$T_{(n_1,n_2,n_3)}\psi_l = e^{i\sum_{i=1}^{3} n_i a_i \frac{2\pi m_{i,l}}{N_i a_i}}\psi_l = e^{i\mathbf{k}_l \cdot \sum_{i=1}^{3} n_i \mathbf{a}_i}\psi_l, \tag{1.60}$$

where we wrote $\mathbf{k}_l = 2\pi \sum_{i=1}^{3} \frac{m_{i,l}}{N_i}\mathbf{b}_i$ in terms of the to $(\mathbf{a}_i)_{i\in(1,2,3)}$ corresponding dual basis $(\mathbf{b}_i)_{i\in(1,2,3)}$. Choosing to write ψ_l as a product of a plane wave $e^{i\mathbf{k}_l\cdot\mathbf{r}}$ and some complex function $u_l(\mathbf{r})$, we obtain

$$e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R_n})}\left(T_\mathbf{n} u\right)(\mathbf{r}) = T_\mathbf{n}\psi_l(\mathbf{r}) = e^{i\mathbf{k}_l\cdot\mathbf{R_n}}\psi_l(\mathbf{r}) = e^{i\mathbf{k}_l\cdot(\mathbf{R_n}+\mathbf{r})}u_l(\mathbf{r}), \tag{1.61}$$

where we wrote $\mathbf{R_n} = \sum_{i=1}^{3} n_i \mathbf{a}_i$. As this holds for any translation, we obtain the result

$$\forall \mathbf{n} \in \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} \colon T_\mathbf{n} u_l = u_l, \tag{1.62}$$

i.e. u_l exhibits the full translational symmetry.

We conclude that any state $\psi \in \mathcal{H}_E$ can be written as a linear combination

$$\psi(\mathbf{r}) = \sum_{l=1}^{\dim \mathcal{H}_E} C_l\ e^{i\mathbf{k}_l\cdot\mathbf{r}}u_l(\mathbf{r}), \tag{1.63}$$

where $\forall\ 1 \leq l \leq \dim \mathcal{H}_E \colon C_l \in \mathbb{C}$.

Note that for any basis vector ψ_l, the choice of $\mathbf{k}_l$ is not unique if not restricting $\mathbf{k}_l$ to the introduced collection of possible choices. In order to see this, consider $\mathbf{k}'_l = \mathbf{K} + \mathbf{k}_l$ where $\forall \mathbf{n} \in \mathbb{Z}_{N_1} \times \mathbb{Z}_{N_2} \times \mathbb{Z}_{N_3} \colon e^{i\mathbf{K}\cdot\mathbf{R_n}} = 1$, in this case the term $e^{i\mathbf{K}\cdot\mathbf{r}}$ can be absorbed into another $u'_l(\mathbf{r}) = e^{-i\mathbf{K}\cdot\mathbf{r}}u_l(\mathbf{r})$ which clearly also exhibits the full translational symmetry.

1.3.2 Reciprocal Lattice and first Brillouin zone

In the literature, the results of Bloch's theorem are often a priori unjustifiedly extended to the case of a spatially indefinitely extended lattice without periodic boundary conditions. This corresponds to the limit of simultaneously diverging N_1, N_2 and N_3 to ∞. This limit however doesn't mathematically exist and thus it is to be borne in mind that we are dealing with a quasi-continuous but actually pure point spectrum which for reasons of simplification

is often treated as if it were continuous.

We define the so-called reciprocal lattice

$$\mathrm{RL} := \left\{ \mathbf{K} \in \mathbb{R}^3 \;\middle|\; \forall \mathbf{R} \in \text{Lattice}\colon e^{i\mathbf{K}\cdot\mathbf{R}} = 1 \right\}. \tag{1.64}$$

On the vector space $\mathbb{R}^3$, we introduce an equivalence relation by

$$\forall \mathbf{k}, \mathbf{k}' \in \mathbb{R}^3\colon\ [\mathbf{k} \sim \mathbf{k}' : \Longleftrightarrow\ \exists \mathbf{K} \in \mathrm{RL}\colon \mathbf{k} - \mathbf{k}' = \mathbf{K}]. \tag{1.65}$$

We can represent the quotient set by the set

$$\left\{ 2\pi \sum_{i=1}^{3} \lambda_i \mathbf{b}_i \;\middle|\; \forall\ 1 \le i \le 3\colon \lambda_i \in [0, 1) \right\}, \tag{1.66}$$

where we, however, will usually exclude 0 from the domain of the λ_i as this is a value which is not attained by any simultaneous eigenstate of the Hamiltonian and all translations. An alternative representation of the quotient set (minus the just mentioned irrelevant boundary) is given by the so-called first Brillouin zone

$$\mathrm{FBZ} := \left\{ \mathbf{k} \in \mathbb{R}^3 \;\middle|\; \forall \mathbf{K} \in \mathrm{RL} \setminus \{0\}\colon |\mathbf{k}| < |\mathbf{k} - \mathbf{K}| \right\}. \tag{1.67}$$

By Bloch's theorem, for any simultaneous eigenstate ψ of the Hamiltonian and all translations, there exists a unique $\mathbf{k}$ in the first Brillouin zone and a unique (up to a constant non-zero factor) periodic function u such that $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$.

1.3.3 Bloch waves visualized

Now let us look at a visualization of a Bloch wave. To this end, we will restrict ourselves to a particle moving in a one-dimensional periodic potential. This will enable us to visualize the wave function $\psi(x)$, plane wave e^{ikx} and $u(x)$ in a 3-dimensional plot.

Suppose we have found a particular solution $\psi(x)$ to some energy E which also is an eigenvector of all translations, just as in the above section. Our solution might look like the complex function depicted on the right hand side of Fig. 1.4. In particular, it might already be periodic with respect to the lattice spacing. Now, according to Bloch's theorem there are several ways to decompose this solution into a product of a plane wave and a lattice-periodic function. There is a unique representation when choosing the wave number k of the plane wave in the first Brillouin zone. In the particular case that is depicted in Fig. 1.4, the wave number would be equal to zero and the periodic function would be equal to the proper eigenfunction $\psi(x)$. We might, however, also absorb all the revolutions across one lattice-spacing

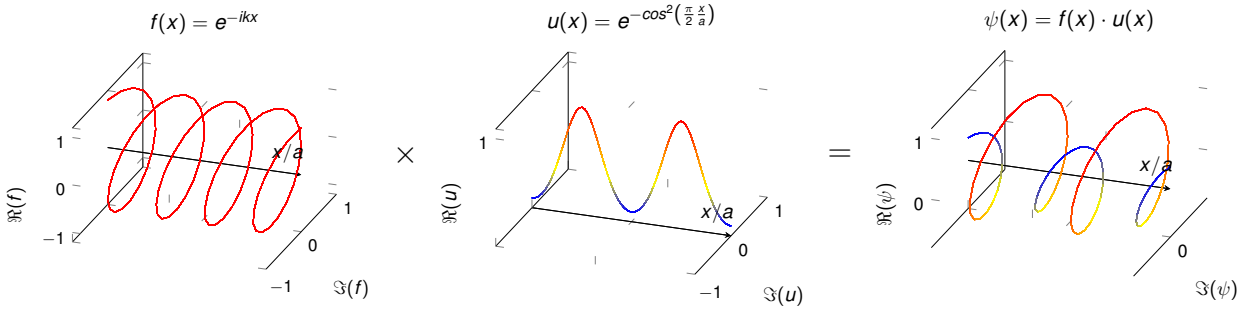

Figure 1.4 Possible decomposition of an eigenvector ψ of the Hamiltonian and all translations into a plane wave e^{ikx} and a lattice-periodic function u. In this case we chose to set the number of total revolutions of u across one lattice-spacing to zero. The domain of the functions covers two lattice-spacings, i.e. $x \in [-a, a]$, for better visualization.

of the $\psi(x)$ into our plane wave e^{ikx} and end up with the composition shown on the left hand side of Fig. 1.4.

1.3.4 Band structure, quasimomentum and effective mass

What we see when explicitly working out the spectrum of H for a specific periodic potential is that we obtain a quasi-continuous band-structure. Once more forgetting about the fact that our $\mathbf{k}$ can only take discrete values, but rather making the already discussed continuum transition, will enable us to introduce the concept of quasiparticles later in this section.

In order to motivate and justify this continuum transition, let us quickly turn to the one-dimensional special case. In the case of a one-dimensional periodic and bounded potential, it is possible to derive Bloch's Theorem without the assumption of periodic boundary conditions. Further, we obtain a strong result which states that the spectrum of the Hamiltonian is an at most countable union of open intervals.

Also, it is possible to easily evaluate the band structure for a given one-dimensional periodic potential. Refer to Fig. 1.5 for an exemplary visualization of the energy bands for an electron in a one-dimensional periodic square-well potential of height $V_0 = 10\,\mathrm{eV}$, thickness $a = 0.5\,\text{Å}$ and lattice-spacing $a + b = 10\,\text{Å}$.

Now let us move back to the general case, however, assuming a continuous spectrum. Suppose we are given some periodic potential V. Let $\mathbf{k}_0$ be a minimum or maximum of a given energy band. Expressing the energy in that band in terms of the so-called quasimomentum $\hbar\mathbf{k}$, we might in particular expand the energy as Taylor series around $\mathbf{k}_0$. Taking into account only terms up to second order (first order vanishes due to $\mathbf{k}_0$ being a minimum or maximum), we

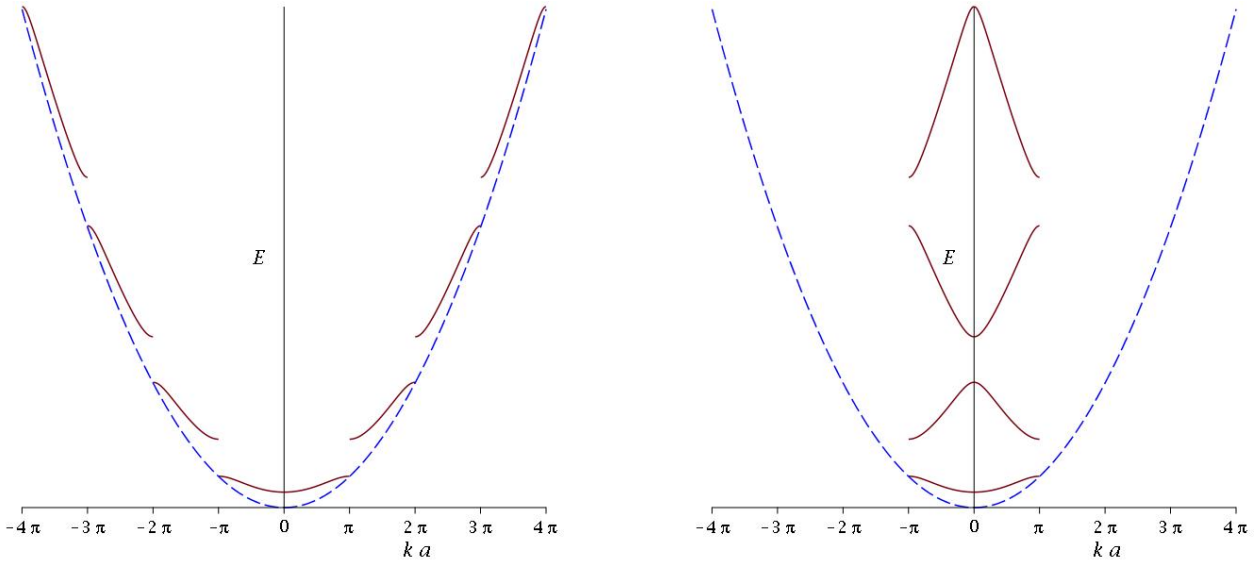

Figure 1.5 Energy bands for an electron in an one-dimensional square-well $V_0 = 10\,\mathrm{eV}$ periodic potential of width $a = 0.5\,\text{Å}$ and spacing $a+b = 10\,\text{Å}$. The energy as a function of the quasimomentum $\hbar k$. On the left hand side, the number of revolutions of the periodic function $u(x)$ is fixed to total zero across one atom-spacing. Identifying the k to some unique $k \in (-\frac{\pi}{a}, \frac{\pi}{a})$ in the first Brillouin zone, the corresponding periodic function $u'(x)$ picks up a finite number of revolutions. As a merit of this identification, energy bands are revealed (right hand side).

can write

$$E_n(\mathbf{k}) = \hbar^2 \sum_{i,j=1}^{3} \left[\frac{1}{2m^*}\right]_{ij} (\mathbf{k}-\mathbf{k}_0)_i (\mathbf{k}-\mathbf{k}_0)_j + E_n(\mathbf{k}_0) + \mathcal{O}\left((\mathbf{k}-\mathbf{k}_0)^3\right), \tag{1.68}$$

where m^* in general is a symmetric tensor, called the effective mass of a particle that in $\mathbf{k}$-space is peaked close to $\mathbf{k}_0$. The above expression clarifies why $\hbar\mathbf{k}$ is often referred to as quasimomentum. Take $1/m^*$ as being proportional to the unit matrix in the chosen basis and $\mathbf{k}_0 = 0$, then we can regard $E_\mathrm{n}(\mathbf{k})$ as the energy of a free (quasi-)particle of effective mass m^* and (quasi-)momentum $\hbar\mathbf{k}$. We can explicitly express m^* as

$$\left[\frac{1}{m^*}\right]_{ij} = \frac{1}{\hbar^2} \left.\frac{\partial^2 E_n}{\partial k_i \partial k_j}\right|_{\mathbf{k}=\mathbf{k}_0}. \tag{1.69}$$

While it is always possible to diagonalize m^* in an orthonormal basis, the effective mass along the main axes are in general not equal. The criterion of validity of the effective mass approximation is in particular met for almost full valence bands or almost empty conduction bands, for which usually $\mathbf{k}_0 = 0$ or some other high-symmetry property for $\mathbf{k}_0$ applies.

Equation (1.69) carries over to a $\mathbf{k}_0$ not corresponding to a minimum or maximum of E_n, for

which it describes how a particle in a state that is peaked around $\mathbf{k}_0$ reacts to external fields.

Depending on the effect one desires to look at, one might average over the three main axes in order to simplify further and to obtain a description which looks like the dispersion relation of a free particle of wave vector $\mathbf{k}$ and scalar mass m^*. The motivation behind this lies entirely in the reduction of the complexity of the problem.

Consider for instance the effect of crystal defects. Using the effective mass approximation, we realize that scattering at a defect for a particle with quasimomentum $\hbar\mathbf{k}$ looks exactly like the scattering of a free particle with momentum $\hbar\mathbf{k}$ and mass m^* at a perturbation which represents the defect, which then, however, would correspond to scattering at an atom instead of a defect.

1.4 Fermi Liquid Theory

We have discussed the motion of a single electron under an arbitrary and a periodic potential. In this section, we are going to consider a system of many electrons. A notable difference here is that statistics should be considered, which makes many-body physics different from a single particle even without interactions. We will discuss this non-interacting Fermi gas at first, and then move forward to the interacting case. Interaction makes the system complicated, and Fermi liquid theory seeks to get rid of the interactions, by replacing interacting electrons with quasi-particles. The striking result is that, near the Fermi surface, quasi-particles behave as free particles, which allows us to apply results of the non-interacting case.

1.4.1 Preliminary: many-body system

Here we follow Nagaosa[10] to introduce the second quatization which is used to deal with a many-body system. We start with the wave function of a many-body system with n particles:

$$\langle \mathbf{r_1}, ..., \mathbf{r_n} | \psi(t) \rangle = \psi(\mathbf{r_1}, ..., \mathbf{r_n}, t). \tag{1.70}$$

The statistics is given by

$$\psi(\mathbf{r_1}, ..., \mathbf{r_i}, ..., \mathbf{r_j}, ..., \mathbf{r_n}, t) = \pm\psi(\mathbf{r_1}, ..., \mathbf{r_j}, ..., \mathbf{r_i}, ..., \mathbf{r_n}, t). \tag{1.71}$$

Here $+$ for bosons and $-$ for fermions. Our goal is to reduce the Hamiltonian to a single-particle form. To do so, we decompose the single particle wavefunction $\psi(\mathbf{r}, t)$ in an orthonor-

mal basis $\phi(\mathbf{r})$:

$$\psi(\mathbf{r},t)=\sum_n a_n(t)\phi(\mathbf{r}). \tag{1.72}$$

Here $\phi(\mathbf{r})$ can be chosen as the eigenstates of the single-particle Hamiltonian H_1 so that it is orthogonal in this basis, which makes life easier.
Now, inserting the above equation into the single-particle Schroedinger equation, we have the time evolution of a_n and a_n^*:

$$\mathrm{i}\hbar\frac{\mathrm{d}a_n(t)}{\mathrm{d}t}=\sum_m\langle\phi_n|H_1|\phi_m\rangle a_m(t) \tag{1.73}$$

$$\mathrm{i}\hbar\frac{\mathrm{d}a_n^*(t)}{\mathrm{d}t}=-\sum_m\langle\phi_m|H_1|\phi_n\rangle a_m^*(t). \tag{1.74}$$

We have also

$$\langle H_1\rangle=\langle\psi(t)|H_1|\psi(t)\rangle=\sum_{n,m}a_n^*(t)a_m(t)\langle\phi_n|H_1|\phi_m\rangle. \tag{1.75}$$

Inserting (1.75) into (1.73) and (1.74), we see that a_n and $\mathrm{i}\hbar a_n^*$ fulfill the canonical equations of $\langle H_1\rangle$:

$$\frac{\mathrm{d}a_n}{\mathrm{d}t}=\frac{\partial\langle H_1\rangle}{\partial(\mathrm{i}\hbar a_n^*)} \tag{1.76}$$

$$\frac{\mathrm{d}(\mathrm{i}\hbar a_n^*)}{\mathrm{d}t}=-\frac{\partial\langle H_1\rangle}{\partial a_n}. \tag{1.77}$$

This motivates us to introduce $\langle H_1\rangle$ as the new Hamiltonian, and a_n, a_n^* to be operators. For N particles, using the normarlized operators $A_n=\sqrt{N}a_n, A_n^\dagger=\sqrt{N}a_n^*$, we can write the many-body Hamiltonian $H=\langle H_1\rangle$ as

$$H=\sum_{n,m}A_n^\dagger\langle\phi_n|H_1|\phi_m\rangle A_m. \tag{1.78}$$

Introducing field operators:

$$\psi^\dagger(\mathbf{r})=\sum_n A_n^\dagger\phi_n^*(\mathbf{r}) \tag{1.79}$$

$$\psi(\mathbf{r})=\sum_n A_n\phi_n(\mathbf{r}), \tag{1.80}$$

we have

$$H = \int \mathrm{d}^3\mathbf{r}\psi^\dagger(\mathbf{r})H_1\psi(\mathbf{r}). \tag{1.81}$$

For a system of non-interacting particles, (1.81) takes the form

$$H = -\int \mathrm{d}^3\mathbf{r}\psi^\dagger(\mathbf{r})\left(\frac{\nabla^2}{2m}\right)\psi(\mathbf{r}), \tag{1.82}$$

or, with a Fourier transfrom,

$$H = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m}\psi^\dagger_{\mathbf{k}}\psi_{\mathbf{k}} = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m}A^\dagger_{\mathbf{k}}A_{\mathbf{k}}. \tag{1.83}$$

Here we use the quasi-momentum $\mathbf{k} = \mathbf{p}/\hbar$, $\mathbf{p}$ being the momentum. From now on we denote $a_{\mathbf{k}} = A_{\mathbf{k}}$, and interpret $a_{\mathbf{k}}$ as the annilation operator on a particle with momentum k. Assume the particle number of the system is not fixed so that we add a chemical potential term, the Hamiltonian we are going to talk about is the Hamiltonian of a **Fermi gas**:

$$H = \sum_{\mathbf{k}} \left(\frac{\hbar^2\mathbf{k}^2}{2m} - \mu\right)a^\dagger_{\mathbf{k}}a_{\mathbf{k}} = \sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)a^\dagger_{\mathbf{k}}a_{\mathbf{k}}. \tag{1.84}$$

For a detailed discussion into second quatization we refer to Nagaosa[10], Altland[11] and Feynman[12].

1.4.2 The theory of Fermi gas

Fermi-surface properties

The Hamiltonian (1.84) tells us that the energy levels of a many-particle system are the same as those of a single-particle, the difference is that here we have many particles occupying different energy levels. The relationship $\epsilon = \epsilon(\mathbf{k})$ is called the dispersion of the particle.
As a result of statistics, any state can not be occupied by two fermions. Thus, even at zero temperature, there are fermions that do not occupy the lowest band. Now if a new fermion wants to enter this system, the lowest possible energy level for it to occupy has an energy greater than the ground state energy, this energy is called the **Fermi-energy**, denoted as ϵ_{F}, or μ. The momentums that satisfy $\epsilon(\mathbf{k}) = \epsilon_{\mathrm{F}}$ form a surface in momentum space, which is called the **Fermi-surface**. Any momentum on this surface are called **Fermi-momentum**, denoted as $\mathbf{k}_{\mathrm{F}}$, the velocity of particles on this surface is $v_{\mathrm{F}} = \frac{\hbar\mathbf{k}_{\mathrm{F}}}{m}$, which is called the **Fermi velocity**.
The Fermi-surface of three dimensional non-interacting fermions is just a sphere with radius

$k_{\mathrm{F}} = |\mathbf{k}_{\mathrm{F}}|$, where

$$k_{\mathrm{F}} = \sqrt{\frac{2m\epsilon_{\mathrm{F}}}{\hbar^2}}. \tag{1.85}$$

The **density of states at Fermi-energy** is given by

$$n(\epsilon_{\mathrm{F}}) = \frac{1}{V}\frac{dN}{d\epsilon}\bigg|_{\epsilon_{\mathrm{F}}}. \tag{1.86}$$

For non-interacting Fermions

$$N = gV\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} = gV\frac{k_{\mathrm{F}}^3}{6\pi^2}, \tag{1.87}$$

where g denotes degeneracy, for electrons there is a spin degeneracy which gives a factor of 2. Inserting (1.87) into (1.86) we find for the Fermi gas

$$n(\epsilon_{\mathrm{F}}) = \frac{mk_{\mathrm{F}}}{\pi^2\hbar}. \tag{1.88}$$

It is striking that many thermodynamic properties, such as specific heat C_v, compressibility κ, and susceptibility χ are only related to the Fermi-surface properties:

$$C_v = \frac{\pi^2 k_B^2 n(\epsilon_{\mathrm{F}})}{3}T \tag{1.89}$$

$$\frac{1}{\kappa} = \frac{2}{3}\frac{N}{V}\epsilon_{\mathrm{F}} \tag{1.90}$$

$$\chi = \frac{1}{2}\mu_B^2 n(\epsilon_{\mathrm{F}}). \tag{1.91}$$

Green's function of a non-interacting fermionic system

The Green's function of a non-interacting fermionic system is given by

$$G_0(\mathbf{k},t) = \begin{cases} -\mathrm{i}\langle\psi|a_{\mathbf{k}}(t)a_{\mathbf{k}}^\dagger(0)|\psi\rangle & t>0 \\ \mathrm{i}\langle\psi|a_{\mathbf{k}}^\dagger(0)a_{\mathbf{k}}(t)|\psi\rangle & t<0 \end{cases}, \tag{1.92}$$

where $|\psi\rangle$ denotes the state of the system.
Setting $\hbar = 1$, the Heisenberg equation of motion of $a_{\mathbf{k}}(t)$ is:

$$\mathrm{i}\frac{\mathrm{d}a_{\mathbf{k}}(t)}{\mathrm{d}t} = [H, a_{\mathbf{k}}(t)]. \tag{1.93}$$

Recalling (1.84), and using $[a_{\mathbf{k}}^{\dagger}(t), a_{\mathbf{k}'}(t)] = \delta_{\mathbf{k},\mathbf{k}'}$, we have

$$a_{\mathbf{k}}(t) = a_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}(\epsilon_{\mathbf{k}}-\mu)t}, \tag{1.94}$$

which gives

$$G_0(\mathbf{k}, t) = \begin{cases} -\mathrm{i}(1-n(\mathbf{k}))\mathrm{e}^{-\mathrm{i}(\epsilon_{\mathbf{k}}-\mu)t} & t > 0 \\ \mathrm{i}n(\mathbf{k})\mathrm{e}^{-\mathrm{i}(\epsilon_{\mathbf{k}}-\mu)t} & t < 0 \end{cases}, \tag{1.95}$$

where $n(\mathbf{k}) = \frac{1}{\mathrm{e}^{\beta(\epsilon_{\mathbf{k}}-\mu)}+1}$ is the number of particles of momentum $\mathbf{k}$ per volume. At zero temperature, $n(\mathbf{k}) = 0$ if $|\mathbf{k}| > k_{\mathrm{F}}$, $n(\mathbf{k}) = 1$ if $|\mathbf{k}| < k_{\mathrm{F}}$.
Taking the Fourier transform with respect to t of (1.95), we have:

$$G_0(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} \mathrm{d}t G_0(\mathbf{k}, t)\mathrm{e}^{\mathrm{i}\omega t} \tag{1.96}$$

$$= \frac{1 - \mathrm{i}\delta_{\mathbf{k}}}{\omega - (\epsilon_{\mathbf{k}} - \mu)} \tag{1.97}$$

$$= \frac{1}{\omega - (\epsilon_{\mathbf{k}} - \mu) + \mathrm{i}\eta_{\mathbf{k}}}, \tag{1.98}$$

where $\delta_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ are infinitesimaly small numbers: $\eta_{\mathbf{k}} > 0$ if $|\mathbf{k}| > k_{\mathrm{F}}$, $\eta_{\mathbf{k}} < 0$ if $|\mathbf{k}| < k_{\mathrm{F}}$.

Conclusion on Fermi gas

The above discussion is carried out at zero temperature. At sufficiently low temperature it also holds. The Fermi gas at sufficiently low temperature is called the degenerate Fermi gas which is sensitive to Pauli-exclusion. On the contrary, at high temperature it forms a dilute Fermi gas, where the Fermi-Dirac statistics can be discribed by the classical Maxwell-Boltzmann statistics.
Compared to single electrons, we have seen the effect of many-body physics in the Fermi gas: statistics has to be considered and Fermi surface arises. However, the Green's function of a Fermi gas is the same as a free electron: after all, the Fermi gas is composed of free electrons. Compared to Fermi gas, we are more interested in fermionic systems with interactions, which are generally not analytically solvable. The **Fermi liquid theory** we are going to discuss seeks to get rid of the interactions in this problem.

1.4.3 Landau's Fermi liquid theory

From now on we deal with electrons subject to electron-electron interaction. The first-quantized Hamiltonian reads:

$$H = H_0 + H_{\text{ee}} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V(\mathbf{r_i} - \mathbf{r_j}). \tag{1.99}$$

Second quantization gives

$$H = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V(\mathbf{q}) a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{k}'}, \tag{1.100}$$

where $V(\mathbf{q}) = \int d\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$ is the Fourier transform of $V(\mathbf{r})$. For electrons in a metal, they interact via the short-ranged Yukawa potential which takes the form

$$V(\mathbf{q}) = \frac{4\pi e^2}{|\mathbf{q}|^2 + k_{\text{TF}}^2}, \tag{1.101}$$

where k_{TF} comes from Thomas-Fermi screening of the Coulomb potential. The short-ranged nature of Yukawa potential makes Landau Fermi liquid theory valid for many metals.
The sum over $\mathbf{q}$ in the second term of (1.100) makes it generally impossible to have an analytic solution of the thermodynamic properties of the system. Landau was first to replace this term with an average field, resulting in free quasi-particles with an effective mass different from that of an electron.

Landau's theory of Fermi liquids

Let us forget about second quantization for a while and follow Landau's approach to Fermi liquid theory in 1956[13]. We consider a degenerate Fermi gas, and gradually turn on a weak interaction between the fermions. This gives the transition from a Fermi gas to a Fermi liquid. The term "gradually" means that this process is **adiabatic**: quantum states and energy levels of Fermi gas are mapped one to one to those of the Fermi liquid.
The energy levels of the Fermi liquid are given by the elementary excitations, called **quasi-particles** of the system. Each quasi-particle possesses a definite momentum, energy, and spin. They obey Fermi-Dirac distribution and their number coincides with that of particles in the Fermi liquid. Landau argued that the quasi-particle can be considered as **a particle in a self-consistent field of surrounding particles**. The energy of a quasi-particle depends on the state of surrounding particles, and the total energy of the whole system is not a simple sum of energies of all individual particles, but a function of the distribution function.
To explicitly see this, let us consider a change in the distribution of quasi-particles $\delta n(\mathbf{p})$,

the corresponding change of the energy of the system is given by

$$\delta E = \sum_{\sigma} \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \epsilon_{\mathbf{p}} \delta n(\mathbf{p}), \tag{1.102}$$

where σ denotes the spin, $\epsilon_{\mathbf{p}} = \delta E/\delta n(\mathbf{p})$ can be regarded as the energy of the added quasi-particle. It is related to the distribution of other quasi-particles since this quasi-particle is in the self-consistent field of surrounding quasi-particles, the change of $\epsilon_{\mathbf{p}}$ with respect to $\delta n(\mathbf{p})$ is

$$\delta \epsilon_{\mathbf{p}} = \sum_{\sigma'} \int \frac{\mathrm{d}^3\mathbf{p}'}{(2\pi\hbar)^3} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') \delta n(\mathbf{p}'), \tag{1.103}$$

where the **Landau response function** $f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')$ is symmetric over $\mathbf{p}$ and $\mathbf{p}'$, and it depends on spins.
Using $\epsilon_{\mathbf{p}}$ we can define the **effective mass** of quasi-particles

$$m^* = p \left(\frac{\partial \epsilon_p}{\partial p} \right)^{-1} \Bigg|_{p=p_F}, \tag{1.104}$$

which is different from that of electrons.

Landau's theory of Fermi liquids in second quantized language

Inserting (1.103) into (1.102), replacing momentum $\mathbf{p}$ with quasi-momentum $\mathbf{k} = \mathbf{p}/\hbar$, we have the **Landau energy functional**

$$\delta E = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k},\sigma} - \mu) a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma,\sigma'} f_{\sigma\sigma'}(\mathbf{k},\mathbf{k}') a^\dagger_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma} a_{\mathbf{k}',\sigma'} \tag{1.105}$$

$$= \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k},\sigma} - \mu) \delta n_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma,\sigma'} f_{\sigma\sigma'}(\mathbf{k},\mathbf{k}') \delta n_{\mathbf{k},\sigma} \delta n_{\mathbf{k}',\sigma'}, \tag{1.106}$$

where we have considered the chemical potential. The dispersion of the quasi-particle is given by

$$\epsilon'_{\mathbf{k},\sigma} = \frac{\delta E}{\delta n_{\mathbf{k},\sigma}} = \epsilon_{\mathbf{k},\sigma} + \frac{1}{V} \sum_{\mathbf{k}',\sigma'} f_{\sigma\sigma'}(\mathbf{k},\mathbf{k}') \delta n_{\mathbf{k}',\sigma'}. \tag{1.107}$$

The second term is the energy of the quasi-particle in the self-consistent field. At low temperatures, this term is proportional to T^2[8], the first term is temperature-independent, thus we can neglect the second term and return to a free particle dispersion $\epsilon_{\mathbf{k},\sigma}$, this time with a

different mass m^* to that of an electron:

$$\epsilon_{\mathbf{k},\sigma} = \frac{\hbar^2 \mathbf{k}^2}{2m^*}. \tag{1.108}$$

The density of states at Fermi-energy is given

$$n(\epsilon_{\mathrm{F}}) = \frac{m^* k_{\mathrm{F}}}{\pi^2 \hbar^2}. \tag{1.109}$$

Now we can derive the thermodynamic properties of a Fermi liquid, noting that $f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}')$ enters κ and χ:

$$C_v = \frac{\pi^2 k_B^2 n(\epsilon_{\mathrm{F}})}{3} T \tag{1.110}$$

$$\frac{1}{\kappa} = \frac{\frac{2}{3}\frac{N}{V}\epsilon_{\mathrm{F}}}{1 + F_0^s} \tag{1.111}$$

$$\chi = \frac{\mu_B^2 n(\epsilon_{\mathrm{F}})}{1 + F_0^a}, \tag{1.112}$$

where (assuming spherical summetry of $f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}')$)

$$f_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') = f^s(\mathbf{k}, \mathbf{k}') + \sigma\sigma' f^a(\mathbf{k}, \mathbf{k}') \tag{1.113}$$

$$F_0^{s,a} = n(\epsilon_{\mathrm{F}}) \int \frac{d\Omega_{\hat{k}'}}{4\pi} f^{s,a}(\hat{k}, \hat{k}'). \tag{1.114}$$

We see that up to some correction with Landau parameters, the thermodynamic properties of a Fermi liquid match that of a Fermi gas.

Lifetime of quasi-particles

Unlike free electrons, quasi-particles are subject to interactions and have a chance to decay. In the following we calculate the lifetime of quasipaerticles. We see that the quasi-particle lifetime is finite and proportional to $(\epsilon_{\mathbf{k}} - \epsilon_{\mathrm{F}})^{-2}$[9].
Consider a quasi-particle at momentum $\mathbf{k}$, after some time it decays into a quasi-particle with momentum $\mathbf{k} - \mathbf{q}$, in the meantime, a quasi-particle below Fermi-energy with momentum $\mathbf{k}'$ will be excited to the state with momentum $\mathbf{k}' + \mathbf{q}$. The inverse lifetime is the sum over rates of all possible decays, given by Fermi's golden rule:

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{2\pi}{\hbar V^2} \sum_{\mathbf{k}',\mathbf{q},s'} |V(\mathbf{q})|^2 n_{0,\mathbf{k}'}(1 - n_{0,\mathbf{k}-\mathbf{q}})(1 - n_{0,\mathbf{k}'+\mathbf{q}}) \delta(\sum \epsilon), \tag{1.115}$$

where $\delta(\sum \epsilon) = \delta(\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}+\epsilon_{\mathbf{k}'+\mathbf{q}})$ gives energy conservation, $n_{0,\mathbf{k}'}(1-n_{0,\mathbf{k}-\mathbf{q}})(1-n_{0,\mathbf{k}'+\mathbf{q}})$ is the Pauli exclusion principle, $V(\mathbf{q})$ is the interaction between quasi-particles.
We consider the three dimensional case, and do the sum over $\mathbf{k}'$ first, Pauli exclusion and energy conservation restricts the number of possible $\mathbf{k}'$s:

$$S(\omega_{\mathbf{q},\mathbf{k}}, q) = \frac{1}{V}\sum_{\mathbf{k}'} n_{0,\mathbf{k}'}(1-n_{0,\mathbf{k}'+\mathbf{q}})\delta(\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}+\epsilon_{\mathbf{k}'+\mathbf{q}}) \tag{1.116}$$

$$= \frac{n(\epsilon_{\mathrm{F}})}{4}\frac{\omega_{\mathbf{q},\mathbf{k}}}{q v_{\mathrm{F}}}, \tag{1.117}$$

where $\hbar\omega_{\mathbf{q},\mathbf{k}} = \hbar^2(2\mathbf{k}\cdot\mathbf{q}-q^2)/2m$. The sum over s' gives a factor of 2, and all we have to do is the sum over $\mathbf{q}$:

$$\frac{1}{V}\sum_{\mathbf{q}} |V(\mathbf{q})|^2 \frac{\omega_{\mathbf{q},\mathbf{k}}}{q} \propto (\epsilon_{\mathbf{k}}-\epsilon_{\mathrm{F}})^2 \int \mathrm{d}q |V(q)|^2. \tag{1.118}$$

For Yukawa potential (1.101) the integral $\int \mathrm{d}q|V(q)|^2$ is finite and we have

$$\frac{1}{\tau_{\mathbf{k}}} \propto (\epsilon_{\mathbf{k}}-\epsilon_{\mathrm{F}})^2. \tag{1.119}$$

We see that **the lifetime of quasi-particle is infinite only when the quasi-particle is near the fermi surface**.
For detailed calculation, the reader is referred to [9].

Green's function of quasi-particles

We will calculate the Green's function of quasi-particles, and expect it to be similar to the Green's function of free electrons (1.98). Recalling (1.92), and noticing that in the interacting case $[H, a_{\mathbf{k},\sigma}(t)]$ takes a rather complicated form, we use the following Heisenberg equation of motion:

$$a_{\mathbf{k},\sigma}(t) = e^{\mathrm{i}Ht} a_{\mathbf{k},\sigma} e^{-\mathrm{i}Ht}. \tag{1.120}$$

In the meantime, we denote the i^{th} energy eigenstate of N interacting particles as $|\psi_i^N\rangle$. It suffices to see that $\sum_m |\psi_m^N\rangle\langle\psi_m^N| = \mathbf{1}$ for all N.
Now, the Green's function is taken on the ground state of an interacting N particle system, using (1.92) and (1.120), we have:

$$G(\mathbf{k},t) = \begin{cases} -\mathrm{i}\langle\psi_0^N|e^{\mathrm{i}E_0^N t} a_{\mathbf{k}} e^{-\mathrm{i}Ht} a_{\mathbf{k}}^\dagger|\psi_0^N\rangle & t>0 \\ \mathrm{i}\langle\psi_0^N|a_{\mathbf{k}}^\dagger e^{\mathrm{i}Ht} a_{\mathbf{k}} e^{-\mathrm{i}E_0^N t}|\psi_0^N\rangle & t<0 \end{cases}. \tag{1.121}$$

For $t > 0$, inserting $\sum_m |\psi_m^{N+1}\rangle\langle\psi_m^{N+1}| = \mathbf{1}$ after e^{-iHt}, we get

$$G(\mathbf{k}, t) = -\mathrm{i}\sum_m |\langle\psi_0^N|a_\mathbf{k}|\psi_m^{N+1}\rangle|^2 e^{-\mathrm{i}(E_m^{N+1}-E_0^N)t}. \tag{1.122}$$

The energy difference $E_m^{N+1} - E_0^N$ is just the energy cost to introduce an extra quasi-particle to the N-particle ground state. The extra particle is added to its m^{th} energy level ϵ_m^{N+1}, s.t. $E_m^{N+1} - E_0^N = \epsilon_m^{N+1} - \mu$. Notice this μ here, since $t > 0$, we require $\epsilon_m^{N+1} - \mu > 0$, s.t. the Fourier transform $G(\mathbf{k}, \omega)$ has poles at $Re(\omega) > 0$, which means this is a possitive-energy solution. Otherwise we will have negative energy for the added particle. This requirement says that if a particle is added to the Fermi sea, it has to be added above the Fermi energy, in agreement with Pauli-exclusion principle.
The Fourier transform of (1.122) gives

$$G(\mathbf{k}, \omega) = \sum_m \frac{|\langle\psi_0^N|a_\mathbf{k}|\psi_m^{N+1}\rangle|^2}{\omega - (\epsilon_m - \mu) + \mathrm{i}\delta_\mathbf{k}}, \tag{1.123}$$

where $\delta_\mathbf{k} > 0$. For Fermi liquid, this complicated sum actually leads to a simple form [3]:

$$G(\mathbf{k}, \omega) = \frac{z_\mathbf{k}}{\omega - (\epsilon_\mathbf{k} - \mu) + \mathrm{i}\eta_\mathbf{k}} + \text{regular part}, \tag{1.124}$$

where $\eta_\mathbf{k} > 0$, $\epsilon_\mathbf{k} = \mathbf{k}^2/2m^*$. The regular part does not contribute to $G(\mathbf{k}, t)$ and can be neglected. This Green's function gives rise to a quasi-particle with dispersion $\omega - (\epsilon_\mathbf{k} - \mu) = 0$. The constant $z_\mathbf{k}$ is called the **quasi-particle weight** and is always less than 1.
Taking account of the quasi-particle-lifetime, the Green's function $G(\mathbf{k}, t)$ decays exponentially with t: $G(\mathbf{k}, t) \propto \exp(-t/\tau_\mathbf{k})$, this gives $\eta_\mathbf{k} \propto 1/\tau_\mathbf{k}$ in (1.124). To really get the Green's function of a free particle, we need $\tau_\mathbf{k} \to \infty$, recalling (1.119), we see that this requires a quasi-particle near Fermi energy. We conclude that **quasi-particles near the Fermi energy behave like free particles**.
For the case $t < 0$, we insert $\sum_m |\psi_m^{N-1}\rangle\langle\psi_m^{N-1}| = \mathbf{1}$. This time we have extracted a quasi-particle, or, in other words, added a quasihole to the Fermi sea. The Green's function for the quasiholes is given by

$$G(\mathbf{k}, \omega) = \frac{z_\mathbf{k}}{\omega - (\epsilon_\mathbf{k} - \mu) - \mathrm{i}\eta_\mathbf{k}}. \tag{1.125}$$

Here $|\epsilon_m - \mu|$ is the energy cost to excite a quasi-particle inside the Fermi sea to the Fermi surface. In all, we can write the Green's function as

$$G(\mathbf{k}, \omega) = \frac{z_\mathbf{k}}{\omega - (\epsilon_\mathbf{k} - \mu) + \mathrm{i}\eta_\mathbf{k}}, \tag{1.126}$$

[3] For detailed calculation, the reader is referred to [14]

where $\eta_{\mathbf{k}} \propto 1/\tau_{\mathbf{k}} \mathrm{sgn}(|\mathbf{k}| - |\mathbf{k}_{\mathrm{F}}|)$. The fact that $z_{\mathbf{k}} < 1$ leads to a modified distribution of quasi-particles at zero temperature, rather than a simple step function (Fig.1.6).

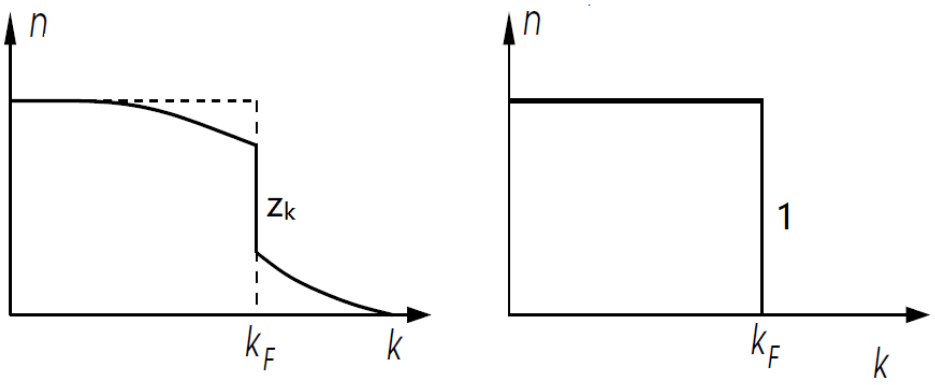

Figure 1.6 Left panel: distribution of quasi-particles at zero temperatre. Right panel: distribution of electrons at zero temperatre.

The jump at k_{F} can be seen as follows:

$$
\begin{aligned}
n(\mathbf{k}) =& \langle a^{\dagger}_{\mathbf{k}}(t) a_{\mathbf{k}}(t) \rangle && (1.127)\\
=& -\mathrm{i} \lim_{t \to 0-} G(\mathbf{k}, t) && (1.128)\\
=& \lim_{t \to 0-} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi \mathrm{i}} G(\mathbf{k}, \omega) e^{-\mathrm{i}\omega t} && (1.129)\\
=& \lim_{t \to 0-} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi \mathrm{i}} \frac{z_{\mathbf{k}}}{\omega - (\epsilon_{\mathbf{k}} - \mu) + \mathrm{i}\eta_{\mathbf{k}}} e^{-\mathrm{i}\omega t}. && (1.130)
\end{aligned}
$$

Since $t < 0$, we close the contour at the upper half-plane when integrating ω. For $k > k_{\mathrm{F}}$, $\eta_{\mathbf{k}} > 0$, the pole of $G(\mathbf{k}, \omega)$ is at the lower half-plane, so (1.130) gives zero. For $k < k_{\mathrm{F}}$, (1.130) is equal to $z_{\mathbf{k}}$, indicating that

$$
\lim_{\epsilon \to 0} n(k_{\mathrm{F}} - \epsilon) - n(k_{\mathrm{F}} + \epsilon) = z_{k_{\mathrm{F}}}. \tag{1.131}
$$

Validicity of Landau's Fermi liquid theory in metals

We want to apply the Fermi liquid theory introduced above to metals. However, a notable difference between metals and the system of intereacting electrons is that in metals we have atoms forming a lattice. The result of having a lattice structure is that the Fermi surface is no longer a sphere as in the above discussion. This, fortunately, does not influence the validicity of Fermi liquid theory. Another influence comes from the phonons provided by the lattice. Below Debye temperature, the electron-phonon interaction dominates, forcing

electrons to form Cooper pairs. At this time the Fermi liquid theory fails. However, for this phenomena to happen one needs very low temperature($\sim 10K$), so this does not affect the validicity of Fermi liquid theory to metals at higher temperatures.
The Fermi liquid theory is not valid in 1D, where instead of forming a Fermi liquid, interacting fermions form a Luttinger liquid. In a Luttinger liquid, the qusiparticle weight z_k vanishes and the distribution $n(k)$ is continuous at k_{F}.
A final remark to add here is that although the above derivation is carried out at low temperture, at high temperature the Fermi liquid theory is still valid as it is at low temperature.

1.5 Conclusion

We started with the general Hamiltonian of a solid and simplified it with the Born-Oppenheimer approximation. In a very first approach, we neglected the electron-electron interaction and considered the scattering of only a single electron at a not yet periodic potential. We applied the method of Green's function on this example and obtained a self-consistent equation: the Lippmann-Schwinger equation. We then made the first Born approximation to obtain a solution for weak scattering potentials and connected this solution to the scattering amplitude and the cross-section. We derived the cross-section explicitly and saw that it was just Rutherford's formula.

We moved on to considering an electron inside a periodic lattice as a simple model of a solid. We experimented with the application of first order perturbation theory in order to see that a periodic potential can no longer be treated as a perturbation to the unperturbed Hamiltonian of a free electron. As a consequence, the problem had to be reconsidered. Exploiting the symmetry of the Hamiltonian led to far-reaching conclusions about the form of eigenwavefunctions, Bloch's theorem. The result suggested us to introduce the concept of quasi-momentum which enabled us to interpret energy-bands. Further we have seen that a particle in an energy-band can under certain conditions be treated as a free quasiparticle with some effective masss m^*. In this picture, the quasi-momentum $\hbar\mathbf{k}$ can be understood as the momentum of the free quasiparticle.

Finally we went to Fermi liquid theory, following Landau's approach, using the simple hypothesis of quasi-particles in a self-consistent field, we are able to treat interacting electrons as non-interacting quasiparticles. This treatment works only for quasiparticles near the Fermi surface. However, this does not restrict our usage of Landau's Fermi liquid theory since we are only interested in the low-energy physics. The Green's function (1.124) of quasiparticles justifies our picture of non-interacting quasiparticles: near the Fermi surface, (1.124) takes

the form of the Green's function of a free fermion, indicating free quasiparticles.
The Fermi liquid theory allows us to treat many metals as non-interacting fermionic systems. From now on we drop the electron-electron interaction and work in the frame of free quasi-particles.

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Chapter 2
Gaussian integrals & supermathematics

Anton Eder [1]

The diagrammatic perturbation approach from previous chapters is well suited for describing conductivity or other response functions, but becomes increasingly tedious for calculating higher order moments. Other phenomena like energy level statistics are completely inaccessible to this formalism. We thus need a new approach: Supersymmetric non-linear sigma models allow for efficient and mathematically rigorous calculation of higher order moments and level statistics. To derive such a model in a consistent way, we have to make use of two new concepts: Gaussian integrals and superlinear algebra. In this chapter, we will provide a short introduction to those mathematical tools, following mainly the book of Efetov [1] and notes by J. Shapiro [2].

2.1 Conductivity on a lattice

The arguably most important transport quantity of a solid is its conductivity σ. Since this chapter focuses on introducing the basic concepts necessary for deriving a non-linear sigma model for the conductivity, it is sufficient to look at σ on an infinite lattice. Although we are ultimately interested in the continuum version of σ, the lattice approach offers the advantage of simplifying most calculations while still capturing all relevant physical phenomena.

2.1.1 Discrete Kubo formula

Suppose that we have a system in equilibrium state ρ_0 and apply a weak perturbation

$$V(t) = -V_0 f(t) A$$

to it, where A is a Hermitian operator and the real function f accounts for the time dependence. To ensure that

$$\lim_{t\to-\infty} \rho(t) = \rho_0$$

[1] supervised by Jacob Shapiro

for the perturbed state $\rho(t)$, we require the perturbation to be turned on *adiabatically*, i.e.

$$\lim_{t\to-\infty} f(t) = 0 \,,$$
$$f(0) = 1 \,.$$

Linear response theory tells us that if we then probe this system with an observable B, its response to $V(t)$ can be described by

$$\begin{aligned} \langle B\rangle_{\rho(t=0)} &= \langle B\rangle_{\rho_0} + \chi_{BA} V_0 + \mathcal{O}(V_0^2) \,, \\ \chi_{BA} &= \mathrm{i}\int_{-\infty}^{0} \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}Ht} B \mathrm{e}^{\mathrm{i}Ht}[A,\rho_0]\right) f(t)\,\mathrm{d}t \ . \end{aligned} \tag{2.1}$$

Since we are interested in the DC conductivity, we take our perturbation to be a weak electric field in x_j-direction

$$V(t) = \boldsymbol{E}\cdot\boldsymbol{x}\,\mathrm{e}^{\varepsilon t} = E_j x_j\,\mathrm{e}^{\varepsilon t}$$

in the limit $\varepsilon \to 0^+$ and probe the system by measuring the current density in x_i-direction

$$j_i = -\operatorname{Tr}\left(v_i\left(\rho(0)-\rho_0\right)\right) = \sigma_{ij}E_j + \mathcal{O}(E_j^2) \,,$$

with $\boldsymbol{v} = \mathrm{i}[H,\boldsymbol{x}]$ referring to the electron velocity. It should be noted that starting from this equation, we have to replace the regular trace $\mathrm{tr}(\,\cdot\,)$ by the *trace per unit volume*

$$\mathrm{Tr}(\,\cdot\,) := \lim_{\Lambda\to\mathbb{Z}^d} \frac{1}{|\Lambda|}\sum_{x\in\Lambda} \langle\delta_x|\ \cdot\ |\delta_x\rangle \ ,$$

since x_k is not a trace class operator. However, all trace properties relevant for this derivation, i.e. linearity and cyclicity, still hold. Assuming that the equilibrium state corresponds to a Fermi-Dirac distribution at zero temperature and Fermi energy E, we can describe ρ_0 in the single-particle picture by the Fermi projection:

$$\rho_0 = \chi_{\leq E}(H) := \lim_{\beta\to\infty}\left(1+\mathrm{e}^{\beta(H-E)}\right)^{-1}$$

After inserting these expressions, equation (2.1) becomes

$$\sigma_{ij}(E) = -\lim_{\varepsilon\to0^+}\int_{-\infty}^{0} \mathrm{Tr}\left(\mathrm{e}^{-\mathrm{i}Ht}\,[H,x_i]\,\mathrm{e}^{\mathrm{i}Ht}\,[x_j,\chi_{\leq E}(H)]\right)\mathrm{e}^{\varepsilon t}\,\mathrm{d}t \ .$$

We can then rewrite

$$\mathrm{e}^{\varepsilon t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{e}^{\varepsilon t}-1}{\varepsilon}\right) \ ,$$

which allows us to perform a partial integration leading to

$$\sigma_{ij}(E) = \lim_{\varepsilon\to 0^+} \int_{-\infty}^{0} \left(\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{Tr}\left(\mathrm{e}^{-\mathrm{i}Ht} \left[H, x_i\right] \mathrm{e}^{\mathrm{i}Ht} \left[x_j, \chi_{\leq E}(H)\right]\right)\right) \frac{\mathrm{e}^{\varepsilon t} - 1}{\varepsilon} \,\mathrm{d}t \ . \tag{2.2}$$

For a derivation avoiding this point please see [3]. Making use of the cyclicity of the trace and the fact that $[H, \rho_0] = 0$, we can express the time derivative by

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{Tr}\left(\mathrm{e}^{-\mathrm{i}Ht} \left[H, x_i\right] \mathrm{e}^{\mathrm{i}Ht} \left[x_j, \chi_{\leq E}(H)\right]\right) &= \operatorname{Tr}\left(\left[H, x_i\right] \frac{\mathrm{d}}{\mathrm{d}t} \left[\mathrm{e}^{\mathrm{i}Ht} x_j \, \mathrm{e}^{-\mathrm{i}Ht}, \chi_{\leq E}(H)\right]\right) \\
&= \operatorname{Tr}\left(\left[H, x_i\right] \mathrm{e}^{\mathrm{i}Ht} \left[\mathrm{i}[H, x_j], \chi_{\leq E}(H)\right] \mathrm{e}^{-\mathrm{i}Ht}\right) \\
&= -\mathrm{i} \operatorname{Tr}\left(v_i \, \mathrm{e}^{\mathrm{i}Ht} \left[v_j, \chi_{\leq E}(H)\right] \mathrm{e}^{-\mathrm{i}Ht}\right) \ .
\end{aligned}$$

We can use the spectral decomposition of H to express functions $f(H)$ as

$$f(H) = \int_{\lambda\in\mathbb{R}} f(\lambda) \,\mathrm{d}P(\lambda) \ ,$$

where P is the projection-valued spectral measure of H. This allows us to move the exponentials - and therefore the time dependence - out of the trace:

$$\begin{aligned}
\operatorname{Tr}\left(v_i \, \mathrm{e}^{\mathrm{i}Ht} \left[v_j, \chi_{\leq E}(H)\right] \mathrm{e}^{-\mathrm{i}Ht}\right) &= \operatorname{Tr}\left(v_i \left(\mathrm{e}^{\mathrm{i}Ht} \, v_j \chi_{\leq E}(H) \, \mathrm{e}^{-\mathrm{i}Ht} - \mathrm{e}^{\mathrm{i}Ht} \, \chi_{\leq E}(H) v_j \, \mathrm{e}^{-\mathrm{i}Ht}\right)\right) \\
&= \int_{(\lambda_1,\lambda_2)\in\mathbb{R}^2} \mathrm{e}^{\mathrm{i}(\lambda_1-\lambda_2)t} \left(\chi_{\leq E}(\lambda_2) - \chi_{\leq E}(\lambda_1)\right) \operatorname{Tr}\left(v_i \,\mathrm{d}P(\lambda_1) \, v_j \,\mathrm{d}P(\lambda_2)\right)
\end{aligned}$$

If we then rewrite

$$\mathrm{e}^{\varepsilon t} - 1 = t \int_0^{\varepsilon} \mathrm{e}^{\eta t} \,\mathrm{d}\eta \ ,$$

we can perform the time integration in equation (2.2):

$$\begin{aligned}
\sigma_{ij}(E) &= \mathrm{i} \lim_{\varepsilon\to 0^+} \int_{\lambda_1,\lambda_2} \int_0^{\varepsilon} \frac{\mathrm{d}\eta}{\varepsilon} \left(\int_{-\infty}^{0} t \, \mathrm{e}^{\mathrm{i}(\lambda_1-\lambda_2-\mathrm{i}\eta)t} \,\mathrm{d}t\right) \left(\chi_{\leq E}(\lambda_1) - \chi_{\leq E}(\lambda_2)\right) \mathrm{d}m_{ij}(\lambda_1,\lambda_2) \\
&= \mathrm{i} \lim_{\varepsilon\to 0^+} \int_{\lambda_1,\lambda_2} \int_0^{\varepsilon} \frac{\mathrm{d}\eta}{\varepsilon} \frac{1}{(\lambda_1 - \lambda_2 - \mathrm{i}\eta)^2} \left(\chi_{\leq E}(\lambda_1) - \chi_{\leq E}(\lambda_2)\right) \mathrm{d}m_{ij}(\lambda_1,\lambda_2) \ ,
\end{aligned}$$

where we defined

$$\mathrm{d}m_{ij}(\lambda_1,\lambda_2) := \operatorname{Tr}\left(v_i \,\mathrm{d}P(\lambda_1) \, v_j \,\mathrm{d}P(\lambda_2)\right) \ .$$

For well-behaved functions f, we can replace

$$\lim_{\varepsilon\to 0^+} \frac{1}{\varepsilon} \int_0^{\varepsilon} f(\eta) \,\mathrm{d}\eta = \lim_{\eta\to 0^+} f(\eta)$$

and with the help of the Sokhotski-Plemelj formula, we find that

$$\begin{aligned}\lim_{\eta\to 0^+}\frac{1}{(t-\mathrm{i}\eta)^2} &= -\frac{\mathrm{d}}{\mathrm{d}t}\lim_{\eta\to 0^+}\frac{1}{t-\mathrm{i}\eta}\\ &= -\left(\mathcal{P}\,\frac{1}{t}\right)' - i\pi\delta'(t)\;.\end{aligned}$$

In this equation, $\mathcal{P}$ refers to the Cauchy principal value. If we assume our system to be time-reversal invariant, one can easily show that

$$\mathrm{d}m_{ij}(\lambda_1,\lambda_2) = \mathrm{d}m_{ij}(\lambda_2,\lambda_1)\,.$$

The product $(\chi_{\leq E}(\lambda_1)-\chi_{\leq E}(\lambda_2))\,\mathrm{d}m_{ij}(\lambda_1,\lambda_2)$ is therefore an *odd* function of (λ_1,λ_2); it follows from symmetry considerations that the integration over the *even* $\mathcal{P}'$-term vanishes and we are left with integrating over the *odd* δ'-function:

$$\begin{aligned}\sigma_{ij}(E) &= \pi\int_{\lambda_1,\lambda_2}\delta'(\lambda_1-\lambda_2)\,(\chi_{\leq E}(\lambda_1)-\chi_{\leq E}(\lambda_2))\,\mathrm{d}m_{ij}(\lambda_1,\lambda_2)\\ &= \pi\int_{\lambda}(\partial_\lambda\,\chi_{\leq E}(\lambda))\,\mathrm{d}m_{ij}(\lambda,\lambda)\end{aligned}$$

At $T=0$, the Fermi distribution is simply a step function around E and we have

$$\partial_\lambda\,\chi_{\leq E}(\lambda) = \partial_\lambda\Theta(E-\lambda) = \delta(E-\lambda)$$

and thus

$$\begin{aligned}\sigma_{ij}(E) &= \pi\int_{\lambda}\delta(E-\lambda)\,\mathrm{Tr}\,(v_i\,\mathrm{d}P(\lambda)\,v_j\,\mathrm{d}P(\lambda))\\ &= \pi\,\partial_{\lambda_1}\partial_{\lambda_2}\,\mathrm{Tr}\,(v_i\,\chi_{\leq\lambda_1}(H)v_j\,\chi_{\leq\lambda_1}(H))\,\Big|_{\lambda_1=\lambda_2=E}\;.\end{aligned}\tag{2.3}$$

We can then make a connection to the Green's function by using Stone's formula (cf. page 237 of [4]) and express the density matrix as

$$\chi_{\leq E}(H) = \lim_{\eta\to 0^+}\frac{1}{\pi}\int_{-\infty}^{E}\mathrm{Im}[R(\epsilon+\mathrm{i}\eta)]\,\mathrm{d}\epsilon = \lim_{\eta\to 0^+}\frac{\eta}{\pi}\int_{-\infty}^{E}|R(\epsilon+\mathrm{i}\eta)|^2\,\mathrm{d}\epsilon\;,\tag{2.4}$$

where $\mathrm{Im}[O] := (O-\overline{O})/2\mathrm{i}$ and R refers to the resolvent of the Hamiltonian:

$$R(z) = (H-z\mathbb{1})^{-1} = \overline{R(\overline{z})}$$

Inserting equation (2.4) into the Kubo formula (2.3) and using the cyclic property of the trace, we obtain

$$\begin{aligned}\sigma_{ij}(E) &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \operatorname{Tr}\left(v_i\, \overline{R(E+\mathrm{i}\eta)} R(E+\mathrm{i}\eta)\, v_j\, R(E+\mathrm{i}\eta)\overline{R(E+\mathrm{i}\eta)}\right) \\ &= -\lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \operatorname{Tr}\left(R(E-\mathrm{i}\eta)[H,x_i]R(E-\mathrm{i}\eta)R(E+\mathrm{i}\eta)[H,x_j]R(E+\mathrm{i}\eta)\right) .\end{aligned}$$

With the useful identity

$$R[H,O]R = [O,R]$$

for any operator O, the above equation simplifies to

$$\sigma_{ij}(E) = -\lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \operatorname{Tr}\left(\left[x_i, R(E-\mathrm{i}\eta)\right]\left[x_j, R(E+\mathrm{i}\eta)\right]\right) .$$

At this point, we can apply Birkhoff's theorem and relate the trace per unit volume to the expectation value $\mathbb{E}[\,\cdot\,]$ of disorder averaging:

$$\begin{aligned}\sigma_{ij}(E) &= -\lim_{\eta\to 0^+} \lim_{\Lambda\to\mathbb{Z}^d} \frac{\eta^2}{\pi|\Lambda|} \sum_{x\in\Lambda} \langle\delta_x| \left[x_i, R(E-\mathrm{i}\eta)\right]\left[x_j, R(E+\mathrm{i}\eta)\right] |\delta_x\rangle \\ &= -\lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \mathbb{E}\left[\langle\delta_0| \left[x_i, R(E-\mathrm{i}\eta)\right]\left[x_j, R(E+\mathrm{i}\eta)\right] |\delta_0\rangle\right]\end{aligned}$$

Since $x_k\,|\delta_0\rangle = 0$, only one term in the expectation value remains:

$$\sigma_{ij}(E) = \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \mathbb{E}\left[\langle\delta_0| R(E-\mathrm{i}\eta) x_i x_j R(E+\mathrm{i}\eta) |\delta_0\rangle\right]$$

and by inserting an identity $\mathbb{1} = \sum_{x\in\mathbb{Z}^d} |\delta_x\rangle\langle\delta_x|$ between the two position operators, we arrive at

$$\begin{aligned}\sigma_{ij}(E) &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \mathbb{E}\left[\sum_{x\in\mathbb{Z}^d} x_i x_j \langle\delta_0| R(E-\mathrm{i}\eta) |\delta_x\rangle \langle\delta_x| R(E+\mathrm{i}\eta) |\delta_0\rangle\right] \\ &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \sum_{x\in\mathbb{Z}^d} x_i x_j\, \mathbb{E}\left[\overline{\langle\delta_x| R(E+\mathrm{i}\eta) |\delta_0\rangle} \langle\delta_x| R(E+\mathrm{i}\eta) |\delta_0\rangle\right] \qquad (2.5) \\ &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \sum_{x\in\mathbb{Z}^d} x_i x_j\, \mathbb{E}\left[|G(x,0;E+\mathrm{i}\eta)|^2\right]\end{aligned}$$

with the Green's function in position basis

$$G(x,y;z) := \langle\delta_x| (H - z\mathbb{1})^{-1} |\delta_y\rangle .$$

This is then our single particle, zero temperature Kubo formula for the DC conductivity on an infinite lattice. This formula and its derivation can also be found in Appendix A of [5].

2.1.2 Green's functions on a finite lattice

To simplify further calculations and get a better understanding of G, we now go to a *finite* lattice Λ, where operators become matrices and we can express the Green's function $G(x, y; E \pm \mathrm{i}\eta)$ as components of an inverse matrix

$$G_\Lambda(x, y; E \pm \mathrm{i}\eta) = \left(\frac{1}{H_\Lambda - (E \pm \mathrm{i}\eta)\mathbb{1}} \right)_{xy} .$$

We can connect our results for the finite lattice back to the Kubo formula (2.5) by using the fact that

$$\lim_{\Lambda \to \mathbb{Z}^d} G_\Lambda(x, y; z) = G(x, y; z) .$$

This is shown in [6]. Depending on the sign of the regulator, G_Λ is either a retarded ("$+\mathrm{i}\eta$") or advanced ("$-\mathrm{i}\eta$") Green's function. This can easily be seen by expressing the Green's function as a Laplace transform:

$$(H - (E \pm \mathrm{i}\eta))^{-1} = \mathrm{i} \int_0^{\pm\infty} \mathrm{e}^{-\mathrm{i}Ht} \mathrm{e}^{\mathrm{i}(E \pm \mathrm{i}\eta)t} \, \mathrm{d}t$$

We choose to model the electron dynamics by a simple Anderson Hamiltonian with a kinetic hopping term and a random potential diagonal in position space:

$$(H_\Lambda)_{xy} = T_{xy} + V_{xy} = \sum_{e \in \Lambda:\, |e|=1} \delta_{x-y,e} + v(x)\, \delta_{xy} , \tag{2.6}$$

where the potential values $v(x)$ are elements of an independent and identically distributed sequence $\{v(x)\}_{x \in \Lambda}$, each drawn with a probability distribution μ on $\mathbb{R}$ (cf. [6]). The main difficulty in evaluating the right-hand side of equation (2.5) now arises from having to average over the inverse of a random potential. However, after introducing both Gaussian integrals and superlinear algebra, we will be able to express G_Λ in a way that allows us to easily take the expectation value.

2.2 Path integrals

In the derivation of our non-linear sigma model, we will be making use of *Gaussian integrals*, which are closely related to *path integrals*. Although these two are not exactly the same, we wish to illustrate some physical principles using the latter before proceeding with the former. To do so, we will follow Chapter 9 of [7]. So far, all quantum calculations were done in the

Hamiltonian formalism, where the time evolution of a state is described by the operator

$$\hat{U} = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}t\right) .$$

The path integral formalism is an equivalent description that makes use of the system's classical Lagrangian instead of its quantum Hamiltonian. In this formalism, one can also easily see how classical mechanics arises from quantum physics.

2.2.1 The action principle in classical mechanics

In classical mechanics, the trajectory $\boldsymbol{q}$ of a particle going from point $\boldsymbol{x}_1 = \boldsymbol{q}(t_1)$ to $\boldsymbol{x}_2 = \boldsymbol{q}(t_2)$ is determined by the *action principle*: Along $\boldsymbol{q}(t)$, the action

$$S\left[\boldsymbol{q}\right] = \int_{t_1}^{t_2} L\left[\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t\right] \,\mathrm{d}t$$

becomes stationary, i.e. its variation vanishes:

$$\delta S\left[\boldsymbol{q}\right] = 0 \tag{2.7}$$

From this condition, we can derive the Euler-Lagrange equations and thus the equations of motion for any classical system, given that we know its Lagrangian L.

2.2.2 The action principle in quantum physics

As it turns out, one can generalize this to a quantum mechanical action principle. Since quantum theory is probabilistic, we now have to talk about transition amplitudes $K(\boldsymbol{x}_1, \boldsymbol{x}_2; t_2 - t_1)$ instead of deterministic trajectories $\boldsymbol{q}$. The probability of the particle going from $\boldsymbol{x}_1$ to $\boldsymbol{x}_2$ in the time interval $t_2 - t_1$ is then given by $|K|^2$. In the path integral formalism, this amplitude is obtained by summing over all possible paths $\boldsymbol{q}(t)$ the particle could take going from $(t_1, \boldsymbol{x}_1)$ to $(t_2, \boldsymbol{x}_2)$, each weighted by a phase factor

$$\exp(\mathrm{i}\varphi[\boldsymbol{q}]) = \exp\left(\mathrm{i}\,\frac{S[\boldsymbol{q}]}{\hbar}\right) .$$

We thus obtain

$$K(\boldsymbol{x}_1, \boldsymbol{x}_2; t_2 - t_1) = \int \mathcal{D}\boldsymbol{q}\; \mathrm{e}^{\mathrm{i}S[\boldsymbol{q}]/\hbar} , \tag{2.8}$$

where the the right-hand side is a functional integration over all allowed paths $\boldsymbol{q}$ obeying the boundary conditions. In non-relativistic quantum mechanics, S is just the classical action

$$S[\boldsymbol{q}] = \int \left(\frac{m}{2}\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q})\right) \mathrm{d}t \ .$$

In quantum field theory, on the other hand, we talk about fields instead of particles, so we have to replace trajectories $\boldsymbol{q} : \mathbb{R} \to \mathbb{R}^3$ by spacetime-dependent field configurations $\phi : \mathbb{R}^4 \to \mathbb{C}^n$; the action along a certain field configuration is then its spacetime-integrated Lagrangian density $\mathcal{L}$:

$$S[\phi] = \int_{\mathbb{R}^4} \mathcal{L}\left[\phi, \partial_\mu \phi, x_\mu\right] \mathrm{d}^4 x$$

The analog of equation (2.8) is therefore

$$K(\phi_1, \phi_2; T) = \langle \phi_2(\boldsymbol{x}, T) | \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}T} \, |\phi_1(\boldsymbol{x}, 0)\rangle = \int \mathcal{D}\phi \, \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}^4 x \, \mathcal{L}[\phi]\right) \ .$$

2.2.3 Connection to classical mechanics

Taking the limit $\hbar \to 0$, the quantum action principle (2.8) becomes equivalent to the classical action principle (2.7). This can be understood intuitively: Paths close to the classical trajectory $\boldsymbol{q}_{\mathrm{cl}}$ all contribute with roughly the same phase φ_{cl}, since $\delta\varphi_{\mathrm{cl}} = \delta S[\boldsymbol{q}_{\mathrm{cl}}]/\hbar = 0$ by definition. The transition probability is thus enhanced by the constructive interference of those paths. Paths further away from $\boldsymbol{q}_{\mathrm{cl}}$, however, vary strongly in S and their phase contributions rotate with period $2\pi\hbar$. Therefore, when summing over those paths, their phases "average out" and one can neglect their contribution. For typical quantum systems, S has order of $\hbar$ and we have to consider many different paths. For classical systems, $S \gg \hbar$ and even slight deviations from $\boldsymbol{q}_{\mathrm{cl}}$ shift the action by $\delta S \gg \hbar$. Consequently, all paths not infinitesimally close to the classical one interfere destructively and the transition probability is determined entirely by the trajectory satisfying the action principle (2.7). More formally, one could also expand in powers of $\hbar$ around $\boldsymbol{q}_{\mathrm{cl}}$ and get quantum corrections corresponding to a WKB approximation.

2.3 Gaussian integrals

While the path integral formalism allows us to express matrix elements $\left(\mathrm{e}^{-\mathrm{i}tH}\right)_{xy}$ of the time evolution operator, the Kubo formula (2.5) requires the Green's function $\left((H - z\mathbb{1})^{-1}\right)_{xy}$. In this section, we will derive a way to express the matrix elements of such inverted operators

via Gaussian integrals. It can be easily shown that for $\varphi \in \mathbb{C}$ and any $a \in \mathbb{C}$ with $\mathrm{Re}[a] > 0$,

$$\frac{1}{\pi} \int_{\mathbb{C}} \mathrm{e}^{-a|\varphi|^2} \, \mathrm{d}\varphi = \frac{1}{a} \, .$$

We are now interested in generalizing this formula for complex vectors $\varphi \in \mathbb{C}^n$ and matrices $A \in \mathbb{C}^{n \times n}$:

$$I_{\mathrm{B}}(A) := \frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle} \, \mathrm{d}\varphi$$

To ensure convergence, A has to have a positive real part $\mathrm{Re}[A] > 0$. Let us also assume that A is unitarily diagonalizable:

$$A = U^\dagger \, \mathrm{diag}(a_1, \ldots, a_n) \, U$$

By substituting $\varphi \to U\tilde{\varphi}$ and using the fact that $|\det(U)| = 1$, we find that

$$\begin{aligned} I_{\mathrm{B}}(A) &= \frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \tilde{\varphi}, \mathrm{diag}(a_1, \ldots, a_n)\tilde{\varphi} \rangle} \, \mathrm{d}\tilde{\varphi} \\ &= \prod_{i=1}^{n} \frac{1}{\pi} \int_{\mathbb{C}} \mathrm{e}^{-a_i |\tilde{\varphi}_i|^2} \, \mathrm{d}\tilde{\varphi}_i \\ &= \prod_{i=1}^{n} \frac{1}{a_i} = \frac{1}{\prod_{i=1}^{n} a_i} \, . \end{aligned}$$

By definition of the determinant, we then have

$$\frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle} \, \mathrm{d}\varphi = \frac{1}{\det(A)} \, . \tag{2.9}$$

One can also show that this is invariant under shifts:

$$\frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi + \alpha, A(\varphi + \beta) \rangle} \, \mathrm{d}\varphi = \frac{1}{\det(A)} \quad \forall \alpha, \beta \in \mathbb{C}^n \tag{2.10}$$

By completing the square and using equation (2.10), we get

$$\frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle + \langle \alpha, \varphi \rangle + \langle \varphi, \beta \rangle} \, \mathrm{d}\varphi = \frac{\mathrm{e}^{\langle \alpha, A^{-1}\beta \rangle}}{\det(A)} \tag{2.11}$$

and have thus found the *partition function* of A with sources α and β, i.e. the *generating functional*

$$Z_{\mathrm{B}}(A; \alpha, \beta) := \frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle + \langle \alpha, \varphi \rangle + \langle \varphi, \beta \rangle} \, \mathrm{d}\varphi \, .$$

Differentiating both sides of equation (2.11) by components $\overline{\alpha_i}$ and β_j and subsequently evaluating them at $\alpha = \beta = 0$, we finally arrive at

$$\frac{1}{\pi^n} \int_{\mathbb{C}^n} \varphi_i \overline{\varphi_j}\, \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \mathrm{d}\varphi = \frac{(A^{-1})_{ij}}{\det(A)} \,. \tag{2.12}$$

With this formula, we are now able to express the inverse of a matrix as a Gaussian integral, which could potentially simplify the disorder averaging in equation (2.5). However, we still have an additional factor of $\det(A)$, which can be highly non-trivial. By combining equations (2.9) and (2.12), we can eliminate this factor:

$$\left(A^{-1}\right)_{ij} = \frac{\int_{\mathbb{C}^n} \varphi_i \overline{\varphi_j}\, \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \mathrm{d}\varphi}{\int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \mathrm{d}\varphi} = \frac{\partial_{\overline{\alpha_i}} \partial_{\beta_j} Z_{\mathrm{B}}(A; \alpha, \beta)}{Z_{\mathrm{B}}(A; 0, 0)} \bigg|_{\alpha=\beta=0}$$

Unfortunately, this normalization brings us back to the initial problem of having to average over the inverse of a random potential; we therefore have to find another way.

2.4 The replica trick

One possible way to do this would be the *replica trick*: Using equation (2.9), we can write

$$1 = \det(A) \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \frac{\mathrm{d}\varphi}{\pi^n}$$

and insert this into equation (2.12) $(N-1)$-times:

$$(A^{-1})_{ij} = \left(\det(A) \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \frac{\mathrm{d}\varphi}{\pi^n} \right)^{N-1} \det(A) \int_{\mathbb{C}^n} \varphi_i \overline{\varphi_j}\, \mathrm{e}^{-\langle \varphi, A\varphi \rangle}\, \frac{\mathrm{d}\varphi}{\pi^n}$$

With Fubini's theorem, we can write this as an integration over N identical replicas $\varphi^{(k)}$ of our system:

$$(A^{-1})_{ij} = \det(A)^N \int_{\mathbb{C}^{nN}} \varphi_i^{(1)} \overline{\varphi_j^{(1)}}\, \mathrm{e}^{-\sum_{k=1}^N \langle \varphi^{(k)}, A\varphi^{(k)} \rangle} \prod_{k=1}^N \frac{\mathrm{d}\varphi^{(k)}}{\pi^n} \quad \forall N \in \mathbb{N} \tag{2.13}$$

The *trick* is to now take the formal limit $N \to 0$:

$$(A^{-1})_{ij} = \lim_{N \to 0} \det(A)^N \int_{\mathbb{C}^{nN}} \varphi_i^{(1)} \overline{\varphi_j^{(1)}}\, \mathrm{e}^{-\sum_{k=1}^N \langle \varphi^{(k)}, A\varphi^{(k)} \rangle} \prod_{k=1}^N \frac{\mathrm{d}\varphi^{(k)}}{\pi^n}$$

If this limit were well-defined, we could take the limit of the first factor and thus eliminate the determinant:

$$(A^{-1})_{ij} = \lim_{N\to 0} \int_{\mathbb{C}^{nN}} \varphi_i^{(1)} \overline{\varphi_j^{(1)}}\, \mathrm{e}^{-\sum_{k=1}^N \langle \varphi^{(k)}, A\varphi^{(k)}\rangle} \prod_{k=1}^N \frac{\mathrm{d}\varphi^{(k)}}{\pi^n}$$

If we were also allowed to interchange the order of disorder averaging and taking the limit, we would have found a way to easily calculate the expectation value:

$$\mathbb{E}\left[(A^{-1})_{ij}\right] = \lim_{N\to 0} \mathbb{E}\left[\int_{\mathbb{C}^{nN}} \varphi_i^{(1)} \overline{\varphi_j^{(1)}}\, \mathrm{e}^{-\sum_{k=1}^N \langle \varphi^{(k)}, A\varphi^{(k)}\rangle} \prod_{k=1}^N \frac{\mathrm{d}\varphi^{(k)}}{\pi^n}\right]$$

However, since the right-hand side of equation (2.13) is only defined for $N \in \mathbb{N}$, it is not clear how the continuous limit $N \to 0$ can be understood. It is also not obvious that $\mathbb{E}[\,\cdot\,]$ and $\lim_{N\to 0}$ can be interchanged. The replica trick is therefore not mathematically rigorous and can in fact lead to wrong results; for more detailed criticism, see [8]. A rigorous alternative to this trick is the *supersymmetry method*, which we will now derive.

2.5 Fermionic integrals

In the previous section, we integrated over complex vectors $\varphi \in \mathbb{C}^n$, whose components φ_x could be interpreted as the values of some (scalar) field at each lattice point $x \in \Lambda$. Since those components are regular *commuting* complex numbers, i.e.

$$\varphi_i \varphi_j = \varphi_j \varphi_i\,,$$

such a field would be of *bosonic* nature. How could we then describe *fermionic* fields? To see this, we have to introduce the concept of anti-commuting variables.

2.5.1 Grassmann numbers

An n-dimensional complex vector space V with an orthonormal basis $\{e_i\}_{i=1}^n$ can be regarded as a $2n$-dimensional real vector space $\tilde{V}$ with a complex structure

$$J : \tilde{V} \to \tilde{V}, \quad J^2 = -\mathbb{1}$$

and an orthonormal basis $\{e_i, Je_i\}_{i=1}^n$. We can use this to define the Grassmannian algebra

$$\mathcal{G}^n := \mathbb{C} \otimes_{\mathbb{R}} \bigwedge \tilde{V}$$

as the complexification of $\bigwedge \tilde{V}$, the 2^{2n}-dimensional exterior algebra over $\tilde{V}$. As such, it has complex dimension 2^{2n} and $2n$ complex generators $\{e_i, Je_i\}_{i=1}^n$. Since we are ultimately interested in describing fermions, it is useful to make a change of basis to

$$\psi_i := \frac{1}{\sqrt{2}} \left(1 \otimes e_i - \mathrm{i} \otimes Je_i\right) ,$$
$$\tilde{\psi}_i := \frac{1}{\sqrt{2}} \left(1 \otimes e_i + \mathrm{i} \otimes Je_i\right) .$$

This way, we get a natural particle anti-particle structure on $\mathcal{G}^n$; both ψ_i and $\tilde{\psi}_i$ are eigenvectors of J and related to each other via complex conjugation:

$$\overline{\psi_i} = \tilde{\psi}_i , \quad \overline{\tilde{\psi}_i} = \psi_i$$

To simplify further definitions, let us label the generators of $\mathcal{G}^n$ more compactly by

$$\{\gamma_i\}_{i=1}^{2n} := \left\{\psi_i, \tilde{\psi}_i\right\}_{i=1}^{n} .$$

A general element of $\mathcal{G}^n$ can then be written as

$$\eta = \sum_{j_1,\ldots,j_{2n}\in\{0,1\}} \alpha_{j_1\ldots j_{2n}} \gamma_1^{j_1} \wedge \ldots \wedge \gamma_{2n}^{j_{2n}} \quad \text{with} \quad \alpha_{j_1\ldots j_{2n}} \in \mathbb{C} , \tag{2.14}$$

where $\wedge$ denotes the exterior product, i.e. the multiplication operation on $\mathcal{G}^n$. A more detailed characterization of $\mathcal{G}^n$ and its structure can be found in Folland's book [9]; for our basic introduction, however, it is sufficient to know that the generators of $\mathcal{G}^n$ *anti-commute*,

$$\gamma_i \wedge \gamma_j = -\gamma_j \wedge \gamma_i , \tag{2.15}$$

making them an obvious choice for representing *fermionic* fields. In particular, this means that their square always vanishes:

$$\gamma_i^2 := \gamma_i \wedge \gamma_i = 0$$

As a consequence, any analytic function of these so-called *Grassmann variables* is a *finite* linear combination of all 2^{2n} basis elements of $\mathcal{G}^n$, given that we interpret the powers in the series representation of such a function as exterior products:

$$\eta^k := \eta^{\wedge k} = \bigwedge_{i=1}^{k} \eta , \quad \eta \in \mathcal{G}^n$$

For our purposes, it is also convenient to define both differentiation and integration on this algebra as linear functionals mapping $\mathcal{G}^n$ to $\mathbb{C}$. Without having to deal with any kind of

limit, we can define an algebraic derivative ∂_{γ_i} by

$$\partial_{\gamma_i} 1 := 0\,,$$
$$\partial_{\gamma_i} \gamma_j := \delta_{ij}$$

and extend this linearly via the generalized Leibniz rule

$$\partial_{\gamma_i}(\eta_1 \wedge \eta_2) := (\partial_{\gamma_i}\eta_1) \wedge \eta_2 + (-1)^{\deg(\eta_1)} \eta_1 \wedge (\partial_{\gamma_i}\eta_2) \tag{2.16}$$

to higher-degree elements as defined in equation (2.14). We also define integration to be the same as differentiation:

$$\int \cdot \; \mathrm{d}\gamma_i := \partial_{\gamma_i} \tag{2.17}$$

Changing the notation back from (γ_i, γ_{i+1}) to $(\psi_i, \tilde{\psi}_i)$, we define:

$$\begin{aligned}\int_{\mathcal{G}^n} \cdot \; \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} &:= \int_{\mathcal{G}^n} \cdot \; \mathrm{d}\psi_1 \wedge \mathrm{d}\tilde{\psi}_1 \wedge \ldots \wedge \mathrm{d}\psi_n \wedge \mathrm{d}\tilde{\psi}_n \\ &= \partial_{\tilde{\psi}_n} \partial_{\psi_n} \ldots \partial_{\tilde{\psi}_1} \partial_{\psi_1}\end{aligned}$$

This can be interpreted as the integration over a fermionic field $\psi = (\psi_1, \ldots, \psi_n)$ and its corresponding antiparticle field $\tilde{\psi} = (\tilde{\psi}_1, \ldots, \tilde{\psi}_n)$ and we find, for example, that

$$\int_{\mathcal{G}^n} 1 \, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} = 0 \quad \text{and} \tag{2.18}$$

$$\int_{\mathcal{G}^n} \psi_1 \wedge \tilde{\psi}_1 \wedge \ldots \wedge \psi_n \wedge \tilde{\psi}_n \, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} = 1\,. \tag{2.19}$$

There also exists a fermionic analog for Fubini's theorem, which can be easily shown with definitions (2.17) and (2.16):

$$\begin{aligned}&\int_{\mathcal{G}^n} F(\gamma_1, \ldots, \gamma_l) \wedge G(\gamma_{l+1}, \ldots, \gamma_{2n}) \, \mathrm{d}\gamma_1 \ldots \mathrm{d}\gamma_{2n} \\ &= (-1)^{(2n-l-1)\deg(\partial_{\gamma_l} \ldots \partial_{\gamma_1} F(\gamma_1, \ldots, \gamma_l))} \left(\int_{\mathcal{G}^{l/2}} F(\gamma_1, \ldots, \gamma_l) \, \mathrm{d}\gamma_1 \ldots \mathrm{d}\gamma_l \right) \\ &\quad \cdot \left(\int_{\mathcal{G}^{n-l/2}} G(\gamma_{l+1}, \ldots, \gamma_{2n}) \, \mathrm{d}\gamma_{l+1} \ldots \mathrm{d}\gamma_{2n} \right)\end{aligned}$$

for functions $F : \mathcal{G}^{l/2} \to \mathcal{G}^n$ and $G : \mathcal{G}^{n-l/2} \to \mathcal{G}^n$. We can also generalize Fubini's theorem to integrals over both bosonic and fermionic variables: For a function $f : X \to \mathcal{G}^n$ mapping some measure space X with measure μ to the Grassmannian algebra $\mathcal{G}^n$, the integral

$$\int_{x \in X} \left(\int_{\mathcal{G}^n} f(x) \, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} \right) \mathrm{d}\mu(x)$$

has a clear interpretation, since

$$\int_{\mathcal{G}^n} f(x)\,\mathrm{d}\psi\,\mathrm{d}\tilde{\psi} \in \mathbb{C} \quad \forall x \in X\ .$$

On the other hand, we may expand any such f in a basis $\{e_i\}_{i=1}^{2^{2n}}$ of $\mathcal{G}^n \cong \mathbb{C}^{2^{2n}}$:

$$f(x) = \sum_{i=1}^{2^{2n}} f_i(x) e_i$$

with coordinate maps $f_i : X \to \mathbb{C}$. Viewing $\mathcal{G}^n$ as a Banach space, we can interpret

$$\int_{x\in X} f(x)\,\mathrm{d}\mu(x) = \sum_{i=1}^{2^{2n}} \left(\int_{x\in X} f_i(x)\,\mathrm{d}\mu(x) \right) e_i \in \mathcal{G}^n$$

as a Bochner integral. The integrals on the right-hand side of this equation are then obviously well-defined. We can thus conclude that

$$\int_{\mathcal{G}^n} \left(\int_{x\in X} f(x)\,\mathrm{d}\mu(x) \right) \mathrm{d}\psi\,\mathrm{d}\tilde{\psi} = \int_{x\in X} \left(\int_{\mathcal{G}^n} f(x)\,\mathrm{d}\psi\,\mathrm{d}\tilde{\psi} \right) \mathrm{d}\mu(x)$$

as long as f is Bochner-integrable.

2.5.2 Fermionic Gaussians

We are now interested in the fermionic equivalent of equation (2.9):

$$I_{\mathrm{F}}(A) := \int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle}\,\mathrm{d}\psi\,\mathrm{d}\tilde{\psi}$$

After defining the bilinear form

$$\langle \psi, A\psi \rangle := \sum_{i,j=1}^{n} A_{ij}\,\tilde{\psi}_i \wedge \psi_j\ ,$$

we can expand the Gaussian up to n-th order (all higher orders vanish because of the anti-commutativity (2.15)):

$$\mathrm{e}^{-\langle \psi, A\psi \rangle} = \sum_{k=0}^{n} \frac{1}{k!} \left(\sum_{i,j=1}^{n} A_{ij}\,\tilde{\psi}_i \wedge \psi_j \right)^{\wedge k}$$

Integrating over ψ and $\tilde{\psi}$, all terms of order smaller than n in the Gaussian also vanish (cf. equation (2.18)) and the integral simplifies to

$$\begin{aligned} I_{\mathrm{F}}(A) &= \int_{\mathcal{G}^n} \frac{1}{n!} \left(\sum_{i,j=1}^{n} A_{ij}\, \tilde{\psi}_i \wedge \psi_j \right)^{\wedge n} \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} \\ &= \int_{\mathcal{G}^n} \frac{(-1)^n}{n!} \sum_{i_1, j_1, \ldots, i_n, j_n = 1}^{n} A_{i_1 j_1} \ldots A_{i_n j_n}\, \tilde{\psi}_{i_1} \wedge \psi_{j_1} \ldots \tilde{\psi}_{i_n} \wedge \psi_{j_n}\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} \end{aligned}$$

Commuting all $\tilde{\psi}_{i_k} \wedge \psi_{j_k}$ to $-\psi_{j_k} \wedge \tilde{\psi}_{i_k}$ and summing over all permutations of i_k, we get an additional factor of $((-1)^n\, n!)$:

$$I_{\mathrm{F}}(A) = \int_{\mathcal{G}^n} \sum_{j_1, \ldots, j_n = 1}^{n} A_{1 j_1} \ldots A_{n j_n}\, \psi_1 \wedge \tilde{\psi}_{j_1} \wedge \ldots \wedge \psi_n \wedge \tilde{\psi}_{j_n}\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi}$$

We then permute the Grassmann variables into the "right" order, giving each term in the sum an additional sign:

$$\begin{aligned} I_{\mathrm{F}}(A) &= \int_{\mathcal{G}^n} \left(\sum_{j_1, \ldots, j_n = 1}^{n} \operatorname{sgn}(\sigma_j) A_{1 j_1} \ldots A_{n j_n} \right) \psi_1 \wedge \tilde{\psi}_1 \ldots \psi_n \wedge \tilde{\psi}_n\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} \\ &= \det(A) \int_{\mathcal{G}^n} \psi_1 \wedge \tilde{\psi}_1 \wedge \ldots \wedge \psi_n \wedge \tilde{\psi}_n\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} \end{aligned}$$

Using equation (2.19), we then finally arrive at our fermionic Gaussian integral:

$$\int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle}\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} = \det(A) \tag{2.20}$$

Comparing this result to equation (2.9), we can see that we again obtain the determinant of A, but this time in the numerator! Analogous to the bosonic case (2.10), one can then show that for any $\eta \in \mathcal{G}^n$,

$$\int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle + \langle \eta, \psi \rangle + \langle \psi, \eta \rangle}\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi} = \det(A)\, \mathrm{e}^{\langle \eta, A^{-1}\eta \rangle}\ . \tag{2.21}$$

We have thus found the *fermionic partition function* of A with source η:

$$Z_{\mathrm{F}}(A; \eta) := \int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle + 2\,\mathrm{Re}[\langle \eta, \psi \rangle]}\, \mathrm{d}\psi\, \mathrm{d}\tilde{\psi}$$

After differentiating both sides of equation (2.21) by $\tilde{\eta}_i$ and η_j and evaluating the result at $\eta = 0$, we find the fermionic equivalent to equation (2.12):

$$\int_{\mathcal{G}^n} \psi_i \wedge \tilde{\psi}_j \, \mathrm{e}^{-\langle \psi, A\psi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi} = \det(A) \, (A^{-1})_{ij} \tag{2.22}$$

To get rid of the determinant factor, we could normalize this expression by inserting equation (2.20):

$$\left(A^{-1}\right)_{ij} = \frac{\int_{\mathcal{G}^n} \psi_i \wedge \tilde{\psi}_j \, \mathrm{e}^{-\langle \psi, A\psi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi}}{\int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi}} = \left. \frac{\partial_{\tilde{\eta}_i} \partial_{\eta_j} Z_{\mathrm{F}}(A;\eta)}{Z_{\mathrm{F}}(A;0)} \right|_{\eta=0}$$

Since this once again brings us back to our inital problem of having to average over the denominator, we have to find a smarter way to eliminate the determinant, for example by integrating over both bosonic *and* fermionic Gaussians. Combining either equations (2.12) and (2.20) or (2.9) and (2.22), we get

$$\begin{aligned} \left(A^{-1}\right)_{ij} &= \left(\int_{\mathcal{G}^n} \mathrm{e}^{-\langle \psi, A\psi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi} \right) \left(\frac{1}{\pi^n} \int_{\mathbb{C}^n} \varphi_i \overline{\varphi_j} \, \mathrm{e}^{-\langle \varphi, A\varphi \rangle} \, \mathrm{d}\varphi \right) \\ &= \left(\frac{1}{\pi^n} \int_{\mathbb{C}^n} \mathrm{e}^{-\langle \varphi, A\varphi \rangle} \, \mathrm{d}\varphi \right) \left(\int_{\mathcal{G}^n} \psi_i \wedge \tilde{\psi}_j \, \mathrm{e}^{-\langle \psi, A\psi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi} \right) . \end{aligned}$$

With Fubini's theorem for mixed integrals, this can be written as

$$\begin{aligned} \left(A^{-1}\right)_{ij} &= \frac{1}{\pi^n} \int_{\mathbb{C}^n} \int_{\mathcal{G}^n} \varphi_i \overline{\varphi_j} \, \mathrm{e}^{-\langle \psi, A\psi \rangle - \langle \varphi, A\varphi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi} \, \mathrm{d}\varphi \\ &= \frac{1}{\pi^n} \int_{\mathbb{C}^n} \int_{\mathcal{G}^n} \psi_i \wedge \tilde{\psi}_j \, \mathrm{e}^{-\langle \psi, A\psi \rangle - \langle \varphi, A\varphi \rangle} \, \mathrm{d}\psi \, \mathrm{d}\tilde{\psi} \, \mathrm{d}\varphi \ . \end{aligned} \tag{2.23}$$

We have thus found a way to overcome our "denominator problem"; to simplify further calculations, however, we have to introduce another new concept.

2.6 Superlinear algebra

Looking at equation (2.23), one can immediately see that it would be very convenient to somehow combine the two fields φ and ψ into a single new field. Indeed, one can define a so-called *supervector*

$$\Phi = \varphi \oplus \psi \in \mathbb{C}^n \oplus \mathcal{G}^n$$

with both bosonic and fermionic components. This is a formal object. Since such supervectors are elements of a highly non-trivial space, we should first examine how concepts from regular linear algebra can be translated to these superspaces.

2.6.1 Linear algebra with anti-commuting scalars

This section follows Chapter 2 of Efetov's book [1]; we will therefore momentarily switch to his notation, which differs slightly from our previous conventions. Most importantly, Efetov defines complex conjugation in such a way that

$$\overline{(\overline{\psi})} = -\psi \ ,$$

while in our convention,

$$\overline{(\overline{\psi})} = \overline{\tilde{\psi}} = \psi \ .$$

Given supervectors of the form

$$\Phi = \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \ ,$$

a general *supermatrix* F acting on such vectors can be written in the following block form:

$$F = \begin{pmatrix} a & \sigma \\ \rho & b \end{pmatrix}$$

Here, a and b are "regular" matrices mapping bosons to bosons and fermions to fermions, while σ and ρ map fermions to bosons and vice versa. It follows, then, that a and b must have commuting components, whereas σ and ρ must have anti-commuting components. We define the *supertranspose* of such a matrix by

$$F^{\mathrm{T}} := \begin{pmatrix} a^{\mathrm{t}} & -\rho^{\mathrm{t}} \\ \sigma^{\mathrm{t}} & b^{\mathrm{t}} \end{pmatrix}$$

with $\cdot^{\mathrm{t}}$ referring to regular transposition $(A^{\mathrm{t}})_{ij} = A_{ji}$. This way, it is ensured that

$$(F_1 F_2)^{\mathrm{T}} = F_2^{\mathrm{T}} F_1^{\mathrm{T}} \ .$$

We should note that in general, $(F^{\mathrm{T}})^{\mathrm{T}} \neq F$; however, defining Hermitian conjugation of supermatrices by

$$F^\dagger := \overline{F^{\mathrm{T}}} \ ,$$

one can easily see that

$$(F_1 F_2)^\dagger = F_2^\dagger F_1^\dagger \ ,$$
$$(F^\dagger)^\dagger = F \ .$$

Taking into account the anticommutativity of the fermionic components of Φ, we define a generalized *supertrace*

$$\mathrm{str}(F) := \mathrm{tr}(a) - \mathrm{tr}(b)$$

that inherits all important properties of the regular trace, e.g. cyclicity:

$$\mathrm{str}(F_1 \dots F_{n-1} F_n) = \mathrm{str}(F_n F_1 \dots F_{n-1})$$

Similarly, we define a *superdeterminant*

$$\mathrm{sdet}(F) := \det\big(a - \sigma b^{-1} \rho\big) \det\big(b^{-1}\big) \ ,$$

which again inherits all properties from its regular variant, e.g. multiplicativity:

$$\mathrm{sdet}(F_1 F_2) = \mathrm{sdet}(F_1)\ \mathrm{sdet}(F_2)$$

We then also maintain the following useful identity:

$$\log(\mathrm{sdet}(F)) = \mathrm{str}(\log(F))$$

Finally, defining the Hermitian conjugate of supervectors by

$$\Phi^\dagger = \overline{\Phi^{\mathrm{t}}} := \big(\overline{\varphi}, \overline{\psi}\big) \ ,$$

one can also define their scalar product

$$\big\langle \Phi^1, \Phi^2 \big\rangle := \Phi^{1\dagger} \Phi^2 = \sum_{i=1}^{2n} \overline{\Phi_i^1} \Phi_i^2 = \sum_{i=1}^{n} \Big(\overline{\varphi_i^1} \varphi_i^2 + \tilde{\psi}_i^1 \wedge \psi_i^2 \Big)$$

and bilinear forms

$$\begin{aligned} \big\langle \Phi^1, F\Phi^2 \big\rangle := \Phi^{1\dagger} F \Phi^2 &= \sum_{i,j=1}^{2n} \overline{\Phi_i^1} F_{ij} \Phi_j^2 \\ &= \sum_{i,j=1}^{n} \Big(\overline{\varphi_i^1} a_{ij} \varphi_j^2 + \overline{\varphi_i^1} \sigma_{ij} \wedge \psi_j^2 + \tilde{\psi}_i^1 \wedge \rho_{ij} \varphi_j^2 + \tilde{\psi}_i^1 \wedge b_{ij} \psi_j^2 \Big) \end{aligned}$$

in the usual manner. These few definitions suffice for our calculations; a more detailed introduction to superlinear algebra can be found in [1].

2.6.2 Gaussian superintegrals

Let us now return to equation (2.23) and our previous notation. Interpreting A as a supermatrix $A \oplus A$, we can condense the two bilinear forms into one:

$$\langle \Phi, A\Phi \rangle = \langle \varphi, A\varphi \rangle + \langle \psi, A\psi \rangle$$

We are also free to define the integration measure on our superspace as

$$\mathrm{d}\Phi := \frac{\mathrm{d}\varphi\,\mathrm{d}\psi\,\mathrm{d}\tilde{\psi}}{\pi^n}$$

and can thus write our inversion formula in the compact form

$$\left(A^{-1}\right)_{ij} = \int \Phi_i^\alpha \overline{\Phi_j^\alpha}\, \mathrm{e}^{-\langle \Phi, A\Phi\rangle}\, \mathrm{d}\Phi \ ,$$

where the index $\alpha \in \{1,2\}$ refers to either the bosonic or fermionic part of Φ and is completely arbitrary (cf. equation (2.23)). Note that there is no implied summation over α. One could then interpret this integral as a field average over a Gaussian distribution determined by the supermatrix A, suggesting the shorthand notation

$$\langle\, \cdot\, \rangle_A := \int \cdot\ \mathrm{e}^{-\langle \Phi, A\Phi\rangle}\, \mathrm{d}\Phi$$

such that we can compactly write

$$\begin{aligned} \langle 1 \rangle_A &= 1 \ , \\ \left\langle \Phi_i^\alpha \overline{\Phi_j^\alpha} \right\rangle_A &= (A^{-1})_{ij} \ . \end{aligned} \tag{2.24}$$

2.7 Taking the disorder average

After introducing these concepts, we can now return to our initial problem of calculating the conductivity. Equipped with the supersymmetric inversion formula (2.24), we can express the electronic Green's functions as

$$\begin{aligned} G_\Lambda(x,y;E \pm \mathrm{i}\eta) &= \left([H_\Lambda - (E \pm \mathrm{i}\eta)\mathbb{1}]^{-1} \right)_{xy} \\ &= \pm \mathrm{i} \left([\eta\mathbb{1} \pm \mathrm{i}(H_\Lambda - E\mathbb{1})]^{-1} \right)_{xy} \\ &= \pm \mathrm{i} \left\langle \Phi_x^\alpha \overline{\Phi_y^\alpha} \right\rangle_{\eta\mathbb{1} \pm \mathrm{i}(H_\Lambda - E\mathbb{1})} \ . \end{aligned}$$

Note that it's necessary to factor out $\pm\mathrm{i}$ to ensure convergence of the integral; since the regulator η is by definition a positive number, this always works. Inserting this back into the expectation value in the Kubo formula (2.5), we find:

$$\begin{aligned} \mathbb{E}\left[|G_\Lambda(x,0;E+\mathrm{i}\eta)|^2 \right] &= \mathbb{E}\left[\overline{G_\Lambda(x,0;E+\mathrm{i}\eta)}\, G_\Lambda(x,0;E+\mathrm{i}\eta) \right] \\ &= \mathbb{E}\left[G_\Lambda(0,x;E-\mathrm{i}\eta)\, G_\Lambda(x,0;E+\mathrm{i}\eta) \right] \\ &= \mathbb{E}\left[\left\langle \Phi_0^\alpha \overline{\Phi_x^\alpha} \right\rangle_{\eta\mathbb{1} - \mathrm{i}(H_\Lambda - E\mathbb{1})} \left\langle \Phi_x^\alpha \overline{\Phi_0^\alpha} \right\rangle_{\eta\mathbb{1} + \mathrm{i}(H_\Lambda - E\mathbb{1})} \right] \end{aligned} \tag{2.25}$$

With the superintegral version of Fubini's theorem, we can then combine these two integrals into one:

$$\begin{aligned}
&\left\langle \Phi_0^\alpha \overline{\Phi_x^\alpha} \right\rangle_{\eta\mathbb{1}-\mathrm{i}(H_\Lambda - E\mathbb{1})} \left\langle \Phi_x^\alpha \overline{\Phi_0^\alpha} \right\rangle_{\eta\mathbb{1}+\mathrm{i}(H_\Lambda - E\mathbb{1})} =: \left\langle \Phi_0^\alpha \overline{\Phi_x^\alpha} \right\rangle_{F^-} \left\langle \Phi_x^\alpha \overline{\Phi_0^\alpha} \right\rangle_{F^+} \\
&= \left(\int \Phi_0^{\alpha-} \overline{\Phi_x^{\alpha-}} \mathrm{e}^{-\left\langle \Phi^-, F^- \Phi^- \right\rangle} \,\mathrm{d}\Phi^- \right) \left(\int \Phi_x^{\alpha+} \overline{\Phi_0^{\alpha+}} \mathrm{e}^{-\left\langle \Phi^+, F^+ \Phi^+ \right\rangle} \,\mathrm{d}\Phi^+ \right) \\
&= \int \Phi_0^{\alpha-} \overline{\Phi_x^{\alpha-}} \Phi_x^{\alpha+} \overline{\Phi_0^{\alpha+}} \mathrm{e}^{-\left\langle \Phi^-, F^- \Phi^- \right\rangle - \left\langle \Phi^+, F^+ \Phi^+ \right\rangle} \,\mathrm{d}\Phi^- \,\mathrm{d}\Phi^+ \\
&= \int \Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \mathrm{e}^{-\langle \Psi, F\Psi \rangle} \,\mathrm{d}\Psi = \left\langle \Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \right\rangle_F \,,
\end{aligned}$$

where we defined a new supervector

$$\Psi := \Phi^- \oplus \Phi^+$$

and a new supermatrix

$$F := F^- \oplus F^+ := [\eta\mathbb{1} - \mathrm{i}(H_\Lambda - E\mathbb{1})] \oplus [\eta\mathbb{1} + \mathrm{i}(H_\Lambda - E\mathbb{1})]$$

such that we can express the modulus square of the Green's function as a single superfield average. Introducing the supermatrix

$$\Lambda := \sigma_3 \otimes \mathbb{1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

(which should not to be confused with the lattice Λ) we can compactly write

$$F = \eta\mathbb{1} - \mathrm{i}\Lambda \otimes (H_\Lambda - E\mathbb{1}) \,.$$

Going back to the impurity average (2.25), one can show that the expectation value and the superintegration $\int \mathrm{d}\Psi$ can be swapped:

$$\begin{aligned}
\mathbb{E}\left[|G_\Lambda(x,0;E+\mathrm{i}\eta)|^2 \right] &= \mathbb{E}\left[\left\langle \Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \right\rangle_F \right] \\
&= \mathbb{E}\left[\int \Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \mathrm{e}^{-\langle \Psi, F\Psi \rangle} \,\mathrm{d}\Psi \right] \\
&= \int \mathbb{E}\left[\Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \mathrm{e}^{-\langle \Psi, F\Psi \rangle} \right] \mathrm{d}\Psi
\end{aligned}$$

and since the superfield components are non-random, we can move them out of the expectation value:

$$\mathbb{E}\left[|G_\Lambda(x,0;E+\mathrm{i}\eta)|^2 \right] = \int \Psi_0^{\alpha-} \overline{\Psi_x^{\alpha-}} \Psi_x^{\alpha+} \overline{\Psi_0^{\alpha+}} \, \mathbb{E}\left[\mathrm{e}^{-\langle \Psi, F\Psi \rangle} \right] \mathrm{d}\Psi \,.$$

We are thus left with the impurity average over the Gaussian; writing out the Hamiltonian (2.6), we find:

$$\begin{aligned}\mathbb{E}\left[\mathrm{e}^{-\langle\Psi,F\Psi\rangle}\right] &= \mathbb{E}\left[\mathrm{e}^{-\langle\Psi,[\eta\mathbb{1}-\mathrm{i}\Lambda\otimes(H_\Lambda-E\mathbb{1})]\Psi\rangle}\right] \\ &= \mathbb{E}\left[\mathrm{e}^{-\langle\Psi,[\eta\mathbb{1}-\mathrm{i}\Lambda\otimes(T_\Lambda-E\mathbb{1})]\Psi\rangle}\ \mathrm{e}^{\mathrm{i}\langle\Psi,(\Lambda\otimes V_\Lambda)\Psi\rangle}\right]\end{aligned}$$

The randomness of the Hamiltonian is contained entirely within the potential term V_Λ; it can therefore be shown that we can also move the non-random Gaussian out of the expectation value:

$$\mathbb{E}\left[\mathrm{e}^{-\langle\Psi,F\Psi\rangle}\right] = \mathrm{e}^{-\langle\Psi,[\eta\mathbb{1}-\mathrm{i}\Lambda\otimes(T_\Lambda-E\mathbb{1})]\Psi\rangle}\ \mathbb{E}\left[\mathrm{e}^{\mathrm{i}\langle\Psi,(\Lambda\otimes V_\Lambda)\Psi\rangle}\right]$$

Using the fact that the potential is diagonal in position basis (cf. equation (2.6)) and the potential values $\{v(x)\}_{x\in\Lambda}$ are *independently* distributed across the lattice sites, we can write

$$\begin{aligned}\mathbb{E}\left[\mathrm{e}^{\mathrm{i}\langle\Psi,(\Lambda\otimes V_\Lambda)\Psi\rangle}\right] &= \mathbb{E}\left[\mathrm{e}^{\mathrm{i}\sum_{x\in\Lambda}v(x)\langle\Psi_x,\Lambda\Psi_x\rangle}\right] \\ &= \prod_{x\in\Lambda}\mathbb{E}\left[\mathrm{e}^{\mathrm{i}v(x)\langle\Psi_x,\Lambda\Psi_x\rangle}\right] =: \prod_{x\in\Lambda}h_x\left(\langle\Psi_x,\Lambda\Psi_x\rangle\right)\ ,\end{aligned} \tag{2.26}$$

where h_x denotes the characteristic function

$$h_x(t) := \int_{v\in\mathbb{R}}\mathrm{e}^{\mathrm{i}vt}\,\mathrm{d}\mu(v) \equiv \mathbb{E}\left[\mathrm{e}^{\mathrm{i}v(x)t}\right]\ \forall x$$

of the distribution μ according to which the potential values $\{v(x)\}_{x\in\Lambda}$ are distributed. Assuming for simplicity that μ is a Gaussian distribution, we find

$$\begin{aligned}h_x(t) &= \int_{v\in\mathbb{R}}\mathrm{e}^{\mathrm{i}vt}\left(\frac{\mathrm{e}^{-\frac{1}{2\sigma_x^2}v^2}}{\sqrt{2\pi}\sigma_x}\,\mathrm{d}v\right) \\ &= \int_{v\in\mathbb{R}}\mathrm{e}^{-\frac{\sigma_x^2}{2}t^2}\left(\frac{\mathrm{e}^{-\frac{1}{2\sigma_x^2}(v-\mathrm{i}\sigma_x^2t)^2}}{\sqrt{2\pi}\sigma_x}\,\mathrm{d}v\right) \\ &= \mathrm{e}^{-\frac{\sigma_x^2}{2}t^2}\int_{v\in\mathbb{R}}\mathrm{d}\mu(v-\mathrm{i}\sigma_x^2t) = \mathrm{e}^{-\frac{\sigma_x^2}{2}t^2}\end{aligned}$$

and our expectation value (2.26) can be written as

$$\begin{aligned}\mathbb{E}\left[\mathrm{e}^{\mathrm{i}\langle\Psi,(\Lambda\otimes V_\Lambda)\Psi\rangle}\right] &= \prod_{x\in\Lambda}\mathrm{e}^{-\frac{\sigma_x^2}{2}\langle\Psi_x,\Lambda\Psi_x\rangle^2} \\ &= \mathrm{e}^{-\sum_{x\in\Lambda}\frac{\sigma_x^2}{2}\langle\Psi_x,\Lambda\Psi_x\rangle^2}\ .\end{aligned}$$

Since the potential values are also *identically* distributed, $\sigma_x = \sigma\ \forall x$ and we get

$$\begin{aligned}\mathbb{E}\left[\mathrm{e}^{\mathrm{i}\langle\Psi,(\Lambda\otimes V_\Lambda)\Psi\rangle}\right] &= \mathrm{e}^{-\frac{\sigma^2}{2}\sum_{x\in\Lambda}\langle\Psi_x,\Lambda\Psi_x\rangle^2} \\ &= \mathrm{e}^{-\frac{\sigma^2}{2}\langle\Psi,\Lambda\Psi\rangle^2}\ .\end{aligned}$$

Finally, we can insert this back into the Kubo formula (2.5):

$$\begin{aligned}\sigma_{ij}(E) &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \sum_{\boldsymbol{x}\in\mathbb{Z}^d} x_i x_j \lim_{\Lambda\to\mathbb{Z}^d} \mathbb{E}\left[|G_\Lambda(x,0;E+\mathrm{i}\eta)|^2\right] \\ &= \lim_{\eta\to 0^+} \frac{\eta^2}{\pi} \sum_{\boldsymbol{x}\in\mathbb{Z}^d} x_i x_j \lim_{\Lambda\to\mathbb{Z}^d} \int \Psi_0^{\alpha-}\overline{\Psi_{\boldsymbol{x}}^{\alpha-}}\Psi_{\boldsymbol{x}}^{\alpha+}\overline{\Psi_0^{\alpha+}} \mathrm{e}^{-\mathcal{F}_\Lambda[\Psi]}\,\mathrm{d}\Psi \ ,\end{aligned}$$

where we defined an "effective action"

$$\begin{aligned}\mathcal{F}_\Lambda[\Psi] &:= -\log\left(\mathbb{E}\left[\mathrm{e}^{-\langle\Psi,F\Psi\rangle}\right]\right) \\ &= \langle\Psi,\left[\eta\mathbb{1}-\mathrm{i}\Lambda\otimes(T_\Lambda-E\mathbb{1})\right]\Psi\rangle + \frac{\sigma^2}{2}\langle\Psi,\Lambda\Psi\rangle^2 \ ,\end{aligned} \tag{2.27}$$

going back to the notion of path integrals. We were thus able to perform the disorder averaging at the cost of introducing a ϕ^4-type self-interaction of our superfield Ψ. To make efficient calculations in the presence of this term, we will have to introduce the concept of non-linear sigma models, which will be the focus of chapter **??**.

2.8 From the lattice to the continuum

This last section is devoted to making the transition from the lattice to the continuum, where our superfields become continuous functions of spacetime, matrices become linear operators and integrals over Ψ become functional integrals:

$$\begin{aligned}(\Psi_x)_{x\in\Lambda} &\to \Psi(\boldsymbol{r}) \\ (H_{xy})_{x,y\in\Lambda} &\to \hat{H} \\ \int \mathrm{d}\Psi &\to \int \mathcal{D}\Psi\end{aligned}$$

Our Gaussian integrals thus change into

$$\langle\,\cdot\,\rangle_F = \int \cdot\ \mathrm{e}^{-\langle\Psi,F\Psi\rangle}\,\mathrm{d}\Psi \to \int \cdot\ \mathrm{e}^{-\int \mathrm{d}\boldsymbol{x}\Psi^\dagger\hat{F}\Psi}\,\mathcal{D}\Psi \ . \tag{2.28}$$

We will also adopt the notation of Efetov and introduce a conjugate field

$$\overline{\Psi} := \Psi^\dagger\Lambda \ ,$$

which should not be confused with complex conjugate of Ψ. We note that the product

$$\overline{\Psi}\Psi = \Psi^\dagger\Lambda\Psi = \Psi^{-\dagger}\Psi^- - \Psi^{+\dagger}\Psi^+$$

is *not* positive definite. Modelling the impurities by a white noise potential, our effective action for the DC conductivity then has the following form:

$$\mathcal{F}_{\mathrm{DC}}[\Psi] = \int \mathrm{d}\boldsymbol{x} \left\{ \eta \Psi^\dagger \Psi - \mathrm{i}\overline{\Psi} \left(\frac{\hat{p}^2}{2m} - E \right) \Psi + \frac{\sigma^2}{2} \left(\overline{\Psi}\Psi \right)^2 \right\}$$

As we can see, this expression is a direct analog to the lattice action (2.27). To make the physics more interesting and establish a connection to Efetov, we want to generalize this action for the AC conductivity. As we have seen many times before, this means we have to introduce an additional frequency dependence to the advanced Green's function:

$$G(x, y; E - \mathrm{i}\eta)\, G(x, y; E + \mathrm{i}\eta) \to G(x, y; E + \omega - \mathrm{i}\eta)\, G(x, y; E + \mathrm{i}\eta)$$

We can account for this by adding a projector

$$P^- = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\mathbb{1} + \Lambda)$$

onto the space of the advanced superfield Ψ^- to our superoperator $\hat{F}$ in equation (2.28):

$$\hat{F}_{\mathrm{DC}} = \begin{pmatrix} \eta - \mathrm{i}(\hat{H} - E) & 0 \\ 0 & \eta + \mathrm{i}(\hat{H} - E) \end{pmatrix} = \eta - \mathrm{i}\Lambda \otimes (\hat{H} - E)$$

$$\to \hat{F}_{\mathrm{AC}} = \begin{pmatrix} \eta - \mathrm{i}(\hat{H} - E + \omega) & 0 \\ 0 & \eta + \mathrm{i}(\hat{H} - E \end{pmatrix} = \eta - \mathrm{i}\left[\Lambda \otimes (\hat{H} - E) + \frac{\omega}{2}(\mathbb{1} + \Lambda) \right]$$

The effective action for the AC conductivity thus becomes

$$\mathcal{F}_{\mathrm{AC}}[\Psi] = \int \mathrm{d}\boldsymbol{x} \left\{ \eta \Psi^\dagger \Psi - \mathrm{i}\overline{\Psi} \left(\frac{\hat{p}^2}{2m} - E + \frac{\omega}{2}(\mathbb{1} + \Lambda) \right) \Psi + \frac{\sigma^2}{2} \left(\overline{\Psi}\Psi \right)^2 \right\} .$$

2.9 Conclusion

Introducing various new concepts like path integrals, Grassmann numbers and supervectors, we were able to express the conductivity of a system as a functional integral over a weighted Gaussian. In contrast to the diagrammatic approach from previous chapters, this allowed us to non-perturbatively calculate the disorder average of σ, albeit at the cost of introducing a ϕ^4-type interaction to our theory, again forcing us to use approximations. To deal with this interaction efficiently, one can use *non-linear sigma models*, which will be introduced in the next chapter.

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Chapter 3

A Non Linear Sigma Model from Conductivity

Jeremy Mann [1]

3.1 A Supersymmetric Field Theory from Conductivity

The aim of this report is to describe the conductivity of disordered metals. If electron-electron interactions are neglected, the one-particle Hamiltonian for the electrons is given by :

$$\hat{H} = \hat{H}_0 + u(\hat{\mathbf{r}}), \tag{3.1}$$

where $\hat{H}_0$ is the Bloch Hamiltonian of the electrons in a potential with lattice periodicity, and $u(\hat{\mathbf{r}})$ is a random potential generated by (non-magnetic) disorder/impurities in the metal.

To simplify calculations, we will use the following model :

1. in the absence of disorder, $\hat{H}_0 = \epsilon(\hat{\mathbf{p}})$ describes a gas of non-interacting Fermionic quasiparticles. At low temperatures, contributions to macroscopic quantities come primarily from quasi-particles at the Fermi sea $\epsilon(\mathbf{p}) = \epsilon_F$.
2. In the continuum limit, $\epsilon(\mathbf{p}) \equiv \frac{\mathbf{p}^2}{2m}$ is the free (quasi-)particle Hamiltonian, with momentum operator $\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}$.
3. The disorder potential is an operator-valued random variable following a "white noise" distribution :
$$\mathbb{E}\left[u(\mathbf{r})\right] = 0 \ , \ \mathbb{E}\left[u(\mathbf{r})u(\mathbf{r}')\right] = \frac{\delta(\mathbf{r}-\mathbf{r}')}{2\pi\nu\tau}. \tag{3.2}$$

This model can be applied to the Fermi liquid theory of metals, where quasi-particles at the Fermi surface are described by the above dispersion with an effective mass m^* (see [1]).

Knowledge of the following physical quantities will be necessary in order to compute the impurity-averaged conductivity :

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- the free density of states $\nu := \frac{\mathrm{d}n}{\mathrm{d}\epsilon}(\epsilon_F)$ at the Fermi surface and the mass m characterizes the quasi-particle dispersion at low temperature in the Fermi Liquid picture.
- The mean free time τ and the mean free path $l = v_F\tau$ provide average time and length scales over which a conduction electron propagates freely in the metal before scattering with an impurity, as reflected in (3.2).

From the Kubo formula, conductivity is proportional to the impurity averaged product of advanced and retarded Green's functions [2, Eq (2.5)], which can be re-expressed using the supersymmetry method as a Gaussian integral over supervector fields Ψ :

$$\mathbb{E}\left[G^A_{\epsilon-\omega}(\mathbf{r},0)G^R_\epsilon(0,\mathbf{r})\right] = \int \mathcal{D}\Psi\, \mathbb{E}\left[e^{-\tilde{F}_\omega[\Psi;u(\mathbf{r})]}\right] \Psi^{1,\alpha}(\mathbf{r})(\Psi^\dagger)^{1,\alpha}(0)\Psi^{2,\beta}(0)(\Psi^\dagger)^{2,\beta}(\mathbf{r}), \tag{3.3}$$

$$\tilde{F}_\omega[\Psi;u] = \int \mathrm{d}\mathbf{r}\, \bar{\Psi}(\mathbf{r})\left\{\Lambda\left(\eta - i\frac{\omega}{2}\right) + i\left(\epsilon - \frac{\omega}{2} - \hat{H}_0 - u(\mathbf{r})\right)\right\}\Psi(\mathbf{r}), \tag{3.4}$$

$$\tag{3.5}$$

where $\bar{\Psi} \equiv \Psi^\dagger\Lambda$ and $\Lambda = \sigma_z^{\mathrm{AR}} \otimes \mathbb{1}^{\mathrm{FB}}$. The AR and FB subscripts denote matrices on advanced/retarded space (Ψ^+, Ψ^-) and Fermion/Boson space (ϕ, χ) respectively.

This allows us to explicitly obtain the impurity-averaged potential contribution $\mathbb{E}\left[e^{-i\int \mathrm{d}\mathbf{r}\, u(\mathbf{r})\bar{\Psi}\Psi}\right] = e^{-\frac{1}{4\pi\nu\tau}\int \mathrm{d}\mathbf{r}\,(\bar{\Psi}\Psi)^2}$. We then obtain an effective action for the supervector field Ψ :

$$\mathbb{E}\left[e^{-\tilde{F}_\omega[\Psi;u]}\right] = e^{-F_\omega[\Psi]}, \tag{3.6}$$

$$F_\omega[\Psi] = \int \mathrm{d}\mathbf{r}\left\{\eta\Psi^\dagger\Psi - i\bar{\Psi}\left(\hat{H}_\omega + \frac{\omega}{2}\Lambda\right)\Psi + \frac{1}{4\pi\nu\tau}(\bar{\Psi}\Psi)^2\right\}, \tag{3.7}$$

where $H_\omega := \hat{H}_0 - \epsilon + \frac{\omega}{2}$. Note that the positive parameter $\eta \to 0^+$ is the regulator initially used to displace the real poles of the advanced and retarded Green's functions to the upper and lower complex plane respectively, thus imposing that the electrons propagate forward in time. Similarly, in the action (3.7), η can also be seen as a "regulator" that ensures the convergence of the path integral (since $\Psi^\dagger\Psi \geq 0$) and correlation functions such as (3.3).

3.2 Analysis of the Effective Action

3.2.1 Decomposition of the Action

At this stage, it is helpful to decompose the effective action into three parts :

$$\begin{aligned} F_\omega[\Psi] &= F_{\text{free}}[\Psi; \epsilon - \omega^+/2] + F_{\text{int}}[\Psi] + \omega^+ F_{\text{ext}}[\psi], \\ F_{\text{free}}[\Psi; E] &= -i \int \mathrm{d}\mathbf{r}\, \bar{\Psi} \left(\hat{H}_0 - E\right) \Psi, \\ F_{\text{int}}[\Psi] &= \frac{i}{4\pi\nu\tau} \int \mathrm{d}\mathbf{r}\, (\bar{\Psi}\Psi)^2, \\ F_{\text{ext}}[\Psi] &= -\frac{i}{2} \int \mathrm{d}\mathbf{r}\, \bar{\Psi}\Lambda\Psi, \end{aligned}$$

where :

1. the **"free" action** $F_{\text{free}}[\Psi; E] = -i \int \mathrm{d}\mathbf{r}\, \bar{\Psi} \left(\hat{H}_0 - E\right) \Psi$ is pure imaginary, thus only changing the phase of the partition weight e^{-F}. F_{free} is stationary for plane waves of energy E, i.e.

$$\delta F_{\text{free}}[\Psi; E]/\delta\bar{\Psi} = 0 \iff \hat{H}_0\Psi = E\Psi. \tag{3.8}$$

   In this case, $E = \epsilon - \omega/2$.

2. The **quartic self-interaction** $F_{\text{int}}[\Psi] = \frac{1}{4\pi\nu\tau} \int \mathrm{d}\mathbf{r}\, (\bar{\Psi}\Psi)^2$ obtained from averaging the phase contributions of the random potential is now a real positive functional, and adds an exponential decay to the partition weight in the path integral. Largest contributions to the path integral will now be those that minimize F_{int} :

$$F_{\text{int}}[\Psi] = \min_{\Psi} F_{\text{int}}[\Psi] = 0 \iff \bar{\Psi}\Psi = 0 \iff |\Psi^-| = |\Psi^+| \tag{3.9}$$

3. The **"external field"** term $\omega^+ F_{\text{ext}}[\Psi] = -i\frac{\omega}{2} \int \mathrm{d}\mathbf{r}\, \bar{\Psi}\Lambda\Psi$ is linear in the AC frequency ω and the regulator η, combined into the complex variable $\omega^+ \equiv \omega + i\eta$. In the limit $\eta \to 0^+$, $\omega F_{\text{ext}}[\Psi]$ is pure imaginary, and its stationary points correspond to supervectors "aligned" with the "external field" $\omega\Lambda$:

$$\delta F_{\text{ext}}[\Psi]/\delta\bar{\Psi} = 0 \iff \omega\Lambda\Psi = \pm\omega\Psi \iff \Psi^+ = 0 \text{ OR } \Psi^- = 0 \tag{3.10}$$

Since $\hat{H}_0 = \hat{\mathbf{p}}^2/2m$ is a scalar in retarded/advanced and Fermion/Boson space, one expects a large degeneracy in saddle point solutions of the DC action $F_{\omega=0}[\Psi]$. However, in the AC case $\omega > 0$, much of the degeneracy in supervector components is lifted by the "external field" matrix Λ.

3.2.2 Symmetry Group of the DC Action

Given an arbitrary saddle point solution $\Psi_T \in \mathcal{M}_\Psi$, any other saddle point $\Psi'_T = V\Psi_T$ can be obtained as the image of Ψ_T by a (supermatrix) symmetry transformation :

$$V \in G_\Psi \iff F_0[V\Psi] = F_0[\Psi]\,, \forall \Psi. \tag{3.11}$$

An arbitrary supermatrix transformation is given by :

$$\begin{aligned}
\Psi &\to V\Psi \\
\bar{\Psi} &\to \bar{\Psi}\bar{V}\,,\ \bar{V} = \Lambda V^\dagger \Lambda \\
F_0[\Psi] &\to F_0[V\Psi] = \int \mathrm{d}\mathbf{r} \left\{ -i\bar{\Psi}\left(\hat{H}_0 - E\right)\bar{V}V\Psi + \frac{1}{4\pi\nu\tau}(\bar{\Psi}\bar{V}V\Psi)^2 \right\} \\
F_{\text{ext}}[\Psi] &\to F_{\text{ext}}[V\Psi] = -\frac{i}{2}\int \mathrm{d}\mathbf{r}\, \bar{\Psi}\bar{V}\Lambda V\Psi
\end{aligned}$$

Therefore, V leaves the DC action F_0 invariant if it conserves the sesquilinear product $\bar{\Psi}\Psi$, i.e. :

$$V \in G \Longleftarrow \bar{V}V = \Lambda V^\dagger \Lambda V = \mathbb{1}. \tag{3.12}$$

On the other hand, $\omega\Lambda$ is "rotated" under V by its adjoint action $\omega\Lambda \to V^{-1}(\omega\Lambda)V$, hence the name "external field" in analogy to SO(3) rotations of external magnetic fields in spin systems. Although we are ultimately interested in the DC limit, the inclusion of the external field term gives us an explicit solution to the saddle point solution (see Sec. 3.2.3) on which to apply the symmetry group transformations in the DC limit.

In addition to supermatrix transformations of the form (3.12), the action (3.7) is also invariant under time reversal symmetry $\mathcal{T}$ (with or without external field term). This discrete symmetry is defined by its action on the (quasi-)electron momentum operator :

$$\mathcal{T} : \hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) \to \hat{H}(-\hat{\mathbf{p}}, \hat{\mathbf{r}}) = \hat{H}(\hat{\mathbf{p}}^{\mathsf{T}}, \hat{\mathbf{r}}) = \hat{H}^{\mathsf{T}}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) \tag{3.13}$$

Where the relation $\hat{\mathbf{p}}^{\mathsf{T}} = -\hat{\mathbf{p}}$ can be obtained using integration by parts. Equivalently, $\mathcal{T}$ can be re-expressed as a supervector transformation :

$$\mathcal{T} : \Psi \to \Psi^*, \tag{3.14}$$

Supermatrix transformations in G_Ψ must therefore preserve time reversal symmetry in addition to (3.12). This condition can be materialized by requiring the external field (as an operator) to remain time reversal invariant after being "rotated" : $(\bar{V}\Lambda V)^{\mathsf{T}} = \bar{V}\Lambda V$.

Alternatively, one can rewrite the 4-component complex supervector as an 8-component real supervector in "time reversal space", that is :

$$\Psi \leftrightarrow \Psi^{\mathrm{TR}} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi \\ \mathcal{T}\Psi \end{pmatrix} = \begin{pmatrix} \Psi \\ \Psi^* \end{pmatrix}. \tag{3.15}$$

In this case, invariance under time reversal can be rewritten as a reality condition in TR space :

$$\Psi^* \leftrightarrow \Psi^{*\mathrm{TR}} \equiv C_0 \Psi^{\mathrm{TR}}, \tag{3.16}$$

where C_0 is a real-valued 8x8 matrix defined by :

$$C_0 \begin{pmatrix} \phi^{\pm} \\ \phi^{*\pm} \end{pmatrix} \equiv \begin{pmatrix} \phi^{*\pm} \\ \phi^{\pm} \end{pmatrix} \ , \ C_0 \begin{pmatrix} \chi^{\pm} \\ \chi^{*\pm} \end{pmatrix} \equiv \begin{pmatrix} \chi^{*\pm} \\ -\chi^{\pm} \end{pmatrix}, \tag{3.17}$$

i.e. $C_0 = \left(J^{\mathrm{TR}} \oplus \sigma_x^{\mathrm{TR}}\right) \otimes \mathbb{1}^{\mathrm{AR}}$, where $J = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ is the symplectic form on the TR space of Grassmann variables. One can then rewrite supermatrices V invariant under time reversal as real-valued 8x8 supermatrices with the reality condition :

$$V^\dagger \leftrightarrow (V^{\mathrm{TR}})^\dagger \equiv C_0 (V^{\mathrm{TR}})^{\mathsf{T}} C_0^{\mathsf{T}} \tag{3.18}$$

The symmetry group G is then given by real 8x8 supermatrices that conserve the bilinear form $C := C_0\Lambda = (J^{\mathrm{TR}} \oplus \sigma_x^{\mathrm{TR}}) \otimes \sigma_z^{\mathrm{AR}}$:

$$V^{\mathrm{TR}} \in G_\Psi \iff V^{\mathrm{TR}} C (V^{\mathrm{TR}})^{\mathsf{T}} = C \tag{3.19}$$

In any case, the adjoint $(...)^\dagger$ and $\overline{(...)}$ operations have the same algebraic properties in 4-dimensional "complex" and 8-dimensional "real" supervector space. As such, the distinction between Ψ and Ψ^{TR} will only be made explicit when the dealing with the domain on which saddle points and their symmetry group are defined. For a more rigorous description of G_Ψ as a Lie supergroup, see [3].

3.2.3 Explicit Saddle Points : Mean Field Approximation

The AC Saddle point

Now that the supermatrix group G moving between saddle points is well defined, we only need to know one explicit saddle point Ψ_T in order to determine a whole orbit $\{V\Psi_T\}_{V\in G_\Psi}$ of other saddle points. Given the similarity of (3.7) with ϕ^4-theories describing spin systems, it make sense to try out the mean field ansatz in this situation as well. This consists of assuming that the quartic self-interaction F_{int} averages to a static (proportional to Λ) external field interaction generated by the mean field solutions, i.e.

$$\int \mathrm{d}\mathbf{r} \left\{ -i\frac{\omega^+}{2}\bar\Psi\Lambda\Psi + \frac{1}{4\pi\nu\tau}(\bar\Psi\Psi)^2 \right\} \longrightarrow -i\frac{\omega_{MF}}{2}\int \mathrm{d}\mathbf{r}\, \bar\Psi_{MF}\Lambda\Psi_{MF}. \tag{3.20}$$

Since the self-interaction is non-negative, the mean field contribution should be a non-negative imaginary term $\Im\{\omega_{MF}\} \geq 0$

After defining the projector field $Q_\Psi := \frac{2}{\pi\nu}\Psi\bar\Psi := \left(\Psi^I\bar\Psi^J\right)_{I,J=(F/B,\pm)}$, the interaction term can be rewritten as :

$$F_{\mathrm{int}}[\Psi] = F_{\mathrm{int}}[Q_\Psi] := \frac{\pi\nu}{16\tau}\int \mathrm{d}\mathbf{r}\, \mathrm{tr}\, Q_\Psi^2, \tag{3.21}$$

where the supertrace operator "tr " is defined by $\mathrm{tr}\, AQ_\Psi := \bar\Psi A\Psi$ for any supermatrix-valued operator A (See Sec. 3.3 for a more general definition). In this form, the ansatz (3.20) is equivalent to a first order expansion of $F_{\mathrm{int}}[Q_\Psi]$ around its mean field average $\langle Q_\Psi\rangle$:

$$\begin{aligned} F_{\text{int}}[\langle Q_\Psi\rangle + \delta Q_\Psi] &= F_{\text{int}}[\langle Q_\Psi\rangle] + \text{tr}\int \mathrm{d}\mathbf{r}\, \delta Q_\Psi \frac{\delta F_\omega}{\delta Q_\Psi}[\langle Q_\Psi\rangle] + \mathcal{O}(\delta Q_\Psi^2) \\ &= F_{\text{int}}[\langle Q_\Psi\rangle] + \frac{\pi\nu}{8\tau}\text{tr}\int \mathrm{d}\mathbf{r}\, \delta Q_\Psi \langle Q_\Psi\rangle + \mathcal{O}(\delta Q_\Psi^2), \end{aligned}$$

with an added constraint that $\langle Q_\Psi\rangle$ be of the same form as the static external field term $\omega\Lambda$:

$$\bar\Psi\left(\omega^+\Lambda + \frac{i}{\tau}\langle Q_\Psi\rangle\right)\Psi \equiv \bar\Psi\left(\omega_{MF}\Lambda\right)\Psi \iff \langle Q_\Psi\rangle \equiv -i\tau(\omega_{MF}-\omega^+)\Lambda \tag{3.22}$$

Since $F_\omega[\langle Q_\Psi\rangle] \propto \text{tr}\,\mathbb{1}, \text{tr}\,\Lambda = 0$, we obtain the mean field action as suggested by (3.20) :

$$F_{MF}[\Psi] := -i\frac{\pi\nu}{2}\int \mathrm{d}\mathbf{r}\,\bar\Psi\left(H_\omega + \frac{1}{2}\omega_{MF}\Lambda\right)\Psi. \tag{3.23}$$

Now, for this ansatz to be consistent, the mean field average $\langle Q_\Psi\rangle = -i\tau(\omega_{MF}-\omega)\Lambda$ around which the action was expanded must correspond to the 2-point function $\frac{2}{\pi\nu}\langle\Psi\bar\Psi\rangle_{F_{MF}[\Psi]}$ averaged with respect to the mean field path integral with action (3.23). Since F_{MF} is quadratic, 2-point functions are given by the inverse of the operator $\hat H_\omega + \frac{\omega_{MF}}{2}\Lambda$. This provides us with a self-consistency equation, often called the **mean field equation**, that determines the value of the mean-field ω_{MF} :

$$\langle Q_\Psi\rangle(\mathbf{r}) = \frac{i}{\pi\nu}\langle\mathbf{r}|\left(\hat H_\omega + \frac{\omega^+}{2}\Lambda + \frac{i}{\tau}\langle Q_\Psi\rangle\right)|\mathbf{r}\rangle = \frac{i}{\pi\nu}\langle\mathbf{r}|\left(\hat H_\omega + \frac{\omega_{MF}}{2}\Lambda\right)|\mathbf{r}\rangle\,. \tag{3.24}$$

With the free Hamiltonian $\hat H_\omega = \frac{\hat{\mathbf{p}}^2}{2m} - \epsilon + \frac{\omega}{2}$ being diagonal in momentum space and Λ diagonal in supervector space, we can rewrite (3.24) in terms of separate $\mathbf{p}$-integrals for each diagonal entry of Λ :

$$\langle Q_\Psi\rangle_{IJ}(\mathbf{r}) = \langle Q_\Psi\rangle_{IJ}(0) = \delta_{IJ}\frac{i}{\pi\nu}\int\frac{\mathrm{d}^d\mathbf{p}}{(2\pi)^d}\left(\xi(\mathbf{p}) + \frac{\omega^+}{2} + \Lambda_{II}\frac{\omega_{MF}}{2}\right)^{-1}, \tag{3.25}$$

where $\xi(\hat{\mathbf{p}}) \equiv \frac{\hat{\mathbf{p}}^2}{2m} - \epsilon$. In Fermi liquid theory, only quasi-particles with momenta $\mathbf{p}$ near the Fermi surface $\epsilon(\mathbf{p}) = \epsilon_F$ contribute to macroscopic quantities, so we can make the approximation $\frac{\mathrm{d}^d\mathbf{p}}{(2\pi)^d} = \mathrm{d}\xi\,\nu(\xi) \simeq \nu\mathrm{d}\xi$. We therefore obtain the equation :

$$\langle Q_\Psi \rangle_{IJ} = \delta_{IJ} \frac{i}{\pi} \int_{\mathbb{R}} \mathrm{d}\xi \, \frac{1}{\xi + \Lambda_{II}\omega_{MF}/2}. \tag{3.26}$$

Assuming $\omega_{MF} \in \mathbb{C} - \mathbb{R}$ is non-real, the integrand in (3.26) has a simple pole which is in the upper complex plane for $\Lambda_{II}\Im\{\omega_{MF}\} > 0$ and the lower complex plane $\Lambda_{II}\Im\{\omega_{MF}\} > 0$. By deforming the contour in upper and lower complex plane respectively, we can apply the residue theorem to obtain :

$$\langle Q_\Psi \rangle_{IJ} = \delta_{IJ} \mathrm{sgn}\left(\Lambda_{II}\Im\{\omega_{MF}\}\right) = \pm\Lambda_{IJ} \tag{3.27}$$

Since $\langle Q_\Psi \rangle \equiv -i\tau(\omega_{MF} - \omega^+)\Lambda$, (3.27) implies $\omega_{MF} \equiv \omega^+ \pm i\tau^{-1}$. Of course, the partition sum $e^{-F_{MF}}$ from (3.23) can only converge if $\Im\{\omega_{MF}\} > 0$, which reduces the mean field solution to :

$$\langle \Psi_{MF}(\mathbf{r})\bar{\Psi}_{MF}(\mathbf{r})\rangle_{F[\Psi]} = \frac{\pi\nu}{2}(\omega^+ + i\tau^{-1})\Lambda. \tag{3.28}$$

There is still a large degeneracy of supervectors Ψ_{MF} satisfying (3.28), the most obvious being related to one another by an arbitrary phase transformation $\Psi_{\mathrm{MF}} \to e^{i\theta}\Psi_{\mathrm{MF}}$. However, it is not necessary to explicitly determine the family of mean-field supervectors satisfying (3.28) to compute physical quantities : since F_{MF} is quadratic in Ψ, all $2n$-point functions are given by products n Green's functions $g_{MF}(\mathbf{r},\mathbf{r}') = \langle \mathbf{r}| \left(\hat{H}_{\omega^+} + \frac{\omega_{MF}}{2}\Lambda\right)^{-1} |\mathbf{r}'\rangle$ using Wick's theorem. In particular, for the four-point functions needed to compute conductivity in (3.3) :

$$\langle \Psi^I(\mathbf{r})\bar{\Psi}^J(0)\Psi^K(0)\bar{\Psi}^L(\mathbf{r})\rangle_{F_{\mathrm{MF}}[\Psi]} = k_{JK} g^{IL}_{MF}(\mathbf{r},\mathbf{r}) g^{KJ}_{MF}(0,0) + g^{IJ}_{MF}(\mathbf{r},0) g^{KL}_{MF}(0,\mathbf{r}), \tag{3.29}$$

where $k = \mathbb{1}^{\mathrm{AR}} \otimes \sigma_z^{\mathrm{FB}} = (-)^{F/B}$ gives a plus/minus sign after permutation of Bosonic/Fermionic fields.

In conclusion, the mean field scheme reduces the self-interaction contribution in (3.23) to a quadratic form $F^{\mathrm{MF}}_{\mathrm{int}}[\Psi] = \frac{\pi\nu}{4\tau}\int \mathrm{d}\mathbf{r}\, \Psi^\dagger\Psi$, assuming negligeable fluctuations of $\Psi\bar{\Psi}$ around its average value (3.28). In particular, this term has the same form as the regularization $\eta\Psi^\dagger\Psi$ in (3.7), which consists in giving a lifetime $\eta^{-1} \to \infty$ to the particles. This approximation is therefore equivalent to a renormalization $\epsilon(\mathbf{p}) \to \epsilon(\mathbf{p}) - i\tau^{-1}$ of the energy spectrum that gives a constant lifetime τ to the particles, namely the **Drude-Boltzmann approximation** previously obtained in the context of perturbation theory using the diagrammatic approach.

Mean Field Saddle Points in the DC Limit

In the absence of external field $\omega = 0$, there is no compelling reason to impose that the mean field generated by the self-interaction be in the same direction as the static field, $\langle Q_\Psi \rangle \propto \Lambda$. We can thus loosen the constraint (3.22) in the first order expansion of (3.21) to obtain the DC mean field ansatz :

$$F_{\mathrm{MF}}[\Psi] = -i\frac{\pi\nu}{2}\int \mathrm{d}\mathbf{r}\, \bar{\Psi}\left(H_{\omega^+} + \frac{i}{2\tau}\langle Q_\Psi\rangle\right)\Psi, \tag{3.30}$$

with $\langle Q_\Psi\rangle(\mathbf{r}) \equiv \text{const}$. Since $\langle Q_\Psi\rangle \to V\langle Q_\Psi\rangle\bar{V}$ is covariant under G for $\Psi \to V\Psi$, the mean field action (3.30) and the mean field equation (3.24) are invariant under G. This implies that solutions to the DC mean field equation (3.24) are obtained by "rotating" the AC mean field Λ by a supermatrix $V \in G_\Psi$:

$$\langle Q_\Psi\rangle = \bar{V}\Lambda V. \tag{3.31}$$

In particular, the set of mean field saddle points for $\langle Q_\Psi\rangle$, $\mathcal{M}_\Psi := \left\{\langle Q_\Psi\rangle = V\Lambda\bar{V}\right\}_{V\in G_\Psi}$ contains the **saddle point manifold** $\mathcal{M} = \{V\Lambda\bar{V}\}_{V\in G} \subset \mathcal{M}_\Psi$, $G \subset G_\Psi$ (see Sec. **??**). In Sec. 3.3.3, we will show that arbitrary saddle points can be expressed as $\mathcal{M}$-valued fields $Q(\mathbf{r}) \in \mathcal{M}$ fluctuating between mean field saddle points on $\mathcal{M}$.

3.3 Supermatrix Action from $F[\Psi]$

The mean field approximation of $F[\Psi]$ suggests that a saddle point analysis at the level of a mean field-type variable $Q \sim \Psi\bar{\Psi}$ can eliminate redundancies and provide explicit parametrizations of the saddle points that dominate the low energy physics in the DC limit. This "variable change" $F[\Psi] \to F[Q]$ can be achieved without any approximation of the form (3.20) using the Hubbard-Stratonovich transformation.

3.3.1 Hubbard-Stratonovich Transformation

The Hubbard-Stratonovich (HS) transformation is a general method used to rewrite an interaction term (in this case $(\bar{\Psi}\Psi)^2$) as an external field term (in this case $\bar{\Psi}Q\Psi$), with an external field $Q(\mathbf{r})$ that is now an extra dynamical variable whose values must be summed over in the path integral.

As an illustration, we will start with a toy model ϕ^4-theory, obtained by reducing the SUSY action (3.7) to only one Bosonic component, i.e. $\Psi \to \phi \in \mathbb{R}$. In this case, the action (with external field $\omega \in \mathbb{R}$) is given by :

$$F_\omega[\phi] = \int \mathrm{d}\mathbf{r} \left\{ -i\phi \left(\frac{\hat{\mathbf{p}}^2}{2m} + \frac{\omega}{2} \right) \phi + \lambda \phi^4 \right\} \tag{3.32}$$

The HS transformation then consists in inserting the gaussian integral $\mathcal{N}^{-1} := \int \mathcal{D}h\, e^{-m^2 \int \mathrm{d}\mathbf{r}\, h^2}$ in the path integral for ϕ :

$$e^{-\lambda \int \mathrm{d}\mathbf{r}\, \phi^4} = \frac{\int \mathcal{D}h\, e^{-\int \mathrm{d}\mathbf{r} \left(m^2 h^2 + \lambda \phi^4 \right)}}{\int \mathcal{D}h\, e^{-m^2 \int \mathrm{d}\mathbf{r}\, h^2}} \tag{3.33}$$

Although h is real-valued, the integration can be shifted into the complex plane by $\mathbb{R} \to \mathbb{R} + i\frac{\sqrt{\lambda}}{m}\phi^2$ without changing the value of the gaussian integral. The ϕ^4-term thus cancels out in favor of an external field term $-i2m\sqrt{\lambda}\phi h \phi$, which allows to rewrite the path integral as :

$$\int \mathcal{D}\phi\, e^{-F_\omega[\phi]} = \mathcal{N} \int \mathcal{D}\phi \int \mathcal{D}h\, e^{-F_{\omega + 2m\sqrt{\lambda}h}[\phi]}, \tag{3.34}$$

where $\mathcal{N}^{-1} = \int \mathcal{D}h\, e^{-m^2 \int \mathrm{d}\mathbf{r}\, h^2}$ is the normalization factor introduced in (3.33).

In conclusino, the HS procedure transforms a quartic interaction term $\lambda\phi(\mathbf{r})^4$ into an external field interaction $\omega(\mathbf{r})\phi(\mathbf{r})^2$, where the external field is is a dynamical variable : $\omega \to \omega(\mathbf{r}) = \omega + 2m\sqrt{\lambda}h(\mathbf{r})$.

The procedure above generalizes in a straightforward way to Grassmannian fields, for instance by reducing (3.7) to one Fermionic component $\Psi \to \chi \in \mathcal{G}$, yielding an action :

$$F_\omega[\chi] = \int \mathrm{d}\mathbf{r} \left\{ -i\chi^* \left(\frac{\hat{\mathbf{p}}^2}{2m} + \frac{\omega}{2} \right) \chi + \lambda (\chi^* \chi)^2 \right\} \tag{3.35}$$

As before, we can introduce the identity $1 = \mathcal{N} \int \mathcal{D}\phi\, e^{-m^2 \int \mathrm{d}\mathbf{r}\, h^2}$ in the path integral and shift the contour by $\mathbb{R} \to \mathbb{R} + i\frac{\sqrt{\lambda}}{m}\chi^*\chi$, ending in (3.34) for the Fermionic path integral $\int \mathcal{D}\chi\, \mathcal{D}\chi^*$.

Going back to the supervector case, we now have a quartic term mixing advanced/retarded and Fermionic/Bosonic fields : $(\bar{\Psi}\Psi)^2 = \left(\phi^{+*}\phi^+ + \chi^{+*}\chi^+ - \phi^{-*}\phi^- - \chi^{-*}\chi^-\right)^2$. In this case, two extra subtleties must be taken into account in the HS procedure $\bar{\Psi}\Psi \to \bar{\Psi} Q \Psi$:

(a) the interaction term now mixes Bosonic and Fermionic fields with quartic terms of the form $\phi^*\phi\chi^*\chi$. Separating these terms requires Fermionic HS fields $Q_{(B,\pm)(F,\pm)} \in \mathcal{G}$.

(b) Instead of performing a separate HS transformation on each separate quartic term in $(\bar{\Psi}\Psi)^2$, one must ensure that the resulting external field term $\bar{\Psi}Q\Psi$ remains invariant under the symmetry group of the initial DC action $F_0[\Psi]$. Therefore, unlike the static external field $\omega\Lambda$, the dynamical external field Q must "rotate" with the supervectors to preserve the symmetry group G_Ψ :

$$\begin{aligned} \Psi &\to V\Psi \\ Q &\to VQ\bar{V} \\ \bar{\Psi}Q\Psi &\to \bar{\Psi}Q\Psi. \end{aligned}$$

In addition, the supermatrix Q should obey a reality condition [2] in order to preserve time-reversal invariance of the action :

$$\overline{\Psi^*}Q\Psi^* = \bar{\Psi}\left(\mathcal{T}Q\mathcal{T}^{-1}\right)\Psi = \bar{\Psi}Q\Psi \Rightarrow \mathcal{T}Q\mathcal{T}^{-1} = \bar{Q} = Q \tag{3.36}$$

In general, (a) implies that Q should be a supermatrix with diagonal Bosonic entries $Q_{FF}, Q_{BB} \in \mathrm{M}_2(\mathbb{C})$ and off-diagonal Fermionic entries $Q_{FB}, Q_{BF} \in \mathrm{M}_2(\mathcal{G})$. Moreover, in order to satisfy (b), it makes the most sense to apply the HS-procedure at the level of the G-invariant sesquilinear product $\bar{\Psi}\Psi$, instead of separate terms $(\Psi^{B/F})^\dagger\Psi^{B/F}$.

In order to achieve this, we first decompose the self-interaction in momentum space :

$$\int \mathrm{d}\mathbf{r}\,(\bar{\Psi}\Psi)^2 = \sum_{\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3+\mathbf{p}_4=0} \bar{\Psi}_{\mathbf{p}_1}\Psi_{\mathbf{p}_2}\bar{\Psi}_{\mathbf{p}_3}\Psi_{\mathbf{p}_4}, \tag{3.37}$$

where $\Psi_{\mathbf{p}} := \mathcal{F}[\Psi](\mathbf{p}) = \int \mathrm{d}\mathbf{r}\, e^{i\mathbf{p}\cdot\mathbf{r}}\Psi(\mathbf{r})$ is the Fourier transform of Ψ, such that $\bar{\Psi}_{\mathbf{p}} \equiv \mathcal{F}[\bar{\Psi}](\mathbf{p}) = \overline{\mathcal{F}[\Psi](-\mathbf{p})} = \overline{\Psi_{-\mathbf{p}}}$.

The constrained sum over the four momenta can be rewritten as a sum over three momenta $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q})$ describing the averaged impurity scattering processes $(\mathbf{p}_1, \mathbf{p}_2) \to (\mathbf{p}_1 \pm \mathbf{q}, \mathbf{p}_2 \mp \mathbf{q})$. Since the mean free path l defines the average distance along which an electron propagates freely between two collisions, we can neglect scattering events at lengths $|\mathbf{q}|^{-1} \equiv q^{-1} \gg l$ that are very unlikely to occur. In this limit, the interaction term can be reexpressed as :

[2] Recall that the condition (3.17) implies $(Q^{\mathrm{TR}})^\dagger = C_0 Q^{\mathrm{TR}} C_0^\intercal$ as Q^{TR} is a supermatrix on TR space.

$$\int \mathrm{d}\mathbf{r}\,(\bar{\Psi}\Psi)^2 \simeq \sum_{q\ll l^{-1}} \Bigg\{ \sum_{\mathbf{p}_1} \left(\bar{\Psi}_{\mathbf{p}_1}\Psi_{-\mathbf{p}_1+\mathbf{q}}\right) \sum_{\mathbf{p}_2} \left(\bar{\Psi}_{\mathbf{p}_2}\Psi_{-\mathbf{p}_2-\mathbf{q}}\right) + \tag{3.38}$$

$$\sum_{\mathbf{p}_1,\mathbf{p}_2} \bar{\Psi}_{\mathbf{p}_1}\Psi_{\mathbf{p}_2} \left(\bar{\Psi}_{-\mathbf{p}_2-\mathbf{q}}\Psi_{-\mathbf{p}_1+\mathbf{q}} + \bar{\Psi}_{-\mathbf{p}_1+\mathbf{q}}\Psi_{-\mathbf{p}_2-\mathbf{q}}\right) \Bigg\} \tag{3.39}$$

It is important to note that without the bound on q, the three terms above would be equal to one another after suitable redefinitions of the sum over $\mathbf{q}$.

The first term (3.38) is "separable" in the sense that it can be written as the (Fourier transform of a) square $a^*_{\mathbf{q}}a_{\mathbf{q}}$ of a scalar $a_{\mathbf{q}} \equiv \sum_{\mathbf{p}} \bar{\Psi}_{\mathbf{p}}\Psi_{-\mathbf{p}+\mathbf{q}} = a^*_{-\mathbf{q}}$ in $\mathbf{q}$-space. We can then perform a HS-transformation using a real scalar $\mathcal{E}$ with momentum space components $\mathcal{E}_{\mathbf{q}} = \mathcal{E}^*_{-\mathbf{q}}$:

$$e^{-\frac{1}{4\pi\nu\tau}\sum_q a^*_{\mathbf{q}}a_{\mathbf{q}}} = \frac{\int \mathcal{D}\mathcal{E}\, e^{-\sum_q \left\{ \frac{\pi\nu}{16\tau}\mathcal{E}^*_{\mathbf{q}}\mathcal{E}_{\mathbf{q}} + \frac{i}{8\tau}\left(a^*_{\mathbf{q}}\mathcal{E}_{\mathbf{q}} + \mathcal{E}^*_{\mathbf{q}}a_{\mathbf{q}}\right)\right\}}}{\int \mathcal{D}\mathcal{E}\, e^{-\frac{\pi\nu}{16\tau}\int \sum_q \mathcal{E}^*_{\mathbf{q}}\mathcal{E}_{\mathbf{q}}}}. \tag{3.40}$$

In real space, the scalar external field term becomes a mass term : $-\frac{i}{8\tau}\sum_{q\ll l^{-1}}\left(a^*_{\mathbf{q}}\mathcal{E}_{\mathbf{q}} + \text{c.c.}\right) \to -\frac{i}{4\tau}\int \mathrm{d}\mathbf{r}\,\mathcal{E}(\mathbf{r})\bar{\Psi}(\mathbf{r})\Psi(\mathbf{r})$, where $\mathcal{E}(\mathbf{r})$ is a slowly fluctuating field. Therefore, in the limit $\epsilon\tau \gg 1 \Rightarrow |\boldsymbol{\nabla}\mathcal{E}| \ll 1$, this interaction term will only contribute by a (quasi-constant) renormalization of the energy $\epsilon \to \epsilon + \frac{\mathcal{E}}{4\tau} \in \mathbb{R}$ without any noticeable contributions to Fermi surface averaged observables.

On the other hand, the second and third terms (3.39) cannot be reduced to scalar interactions in $\mathbf{q}$-space, and the HS-transformation can only be achieved with a full supermatrix field $Q(\mathbf{r})$. It is interesting to note that these two terms are related to one another by time reversal [3], thus suggesting their interpretation as the impurity-averaged Diffuson and Cooperon interactions. In any case, a re-ordering of the $\mathbf{p}_{1,2}$ sums shows that these terms are equal to one another in the SUSY formalism [4], and can be "separated" as in (3.38), but only as the supertrace of a matrix product $\mathrm{tr}\bar{A}_{\mathbf{q}}A_{\mathbf{q}}$ in $\mathbf{q}$-space, where $A_{\mathbf{q}} := \sum_{\mathbf{p}} \Psi_{\mathbf{p}}\bar{\Psi}_{-\mathbf{p}+\mathbf{q}} = \overline{A_{-\mathbf{q}}}$. Since $A_{\mathbf{q}}$ transforms like (b) under V and $\mathcal{T}$, the HS transformation can be done with a supermatrix Q of the same type as $A_{\mathbf{q}}$, and more generally transforming like $Q \sim \Psi\bar{\Psi}$ under G_Ψ.

Naively, one would expect to obtain the same expression as (3.40) using the prescription $(a_{\mathbf{q}}, \mathcal{E}, \mathcal{E}_{-\mathbf{q}}a_{\mathbf{q}}) \to (A_{\mathbf{q}}, Q, \mathrm{tr}\, Q_{-\mathbf{q}}A_{\mathbf{q}})$. While this formally provides the final result, the domain of the supermatrix components Q_{IJ} will have to be different than that of $\mathcal{E} \in \mathbb{R}$ in order to

[3] since $\bar{\Psi}^*_1\Psi^*_2 = (\bar{\Psi}_2\Psi_1)^{\mathsf{T}} = \bar{\Psi}_2\Psi_1$, and $\mathcal{T}\Psi = \Psi^*$.

[4] In the absence of time-reversal breaking interactions.

ensure the convergence of the identity element $1 = \int \mathcal{D}Q\, e^{-\frac{\pi\nu}{16\tau}\mathrm{tr}\sum_q Q^*_{\mathbf{q}}Q_{\mathbf{q}}}$ inserted in the HS transformation. This comes from the important caveat that the supertrace of a square is **not non-negative** :

$$\mathrm{tr}\, Q^2 = \mathrm{tr}\, Q^2_{FF} - \mathrm{tr}\, Q^2_{BB} \tag{3.41}$$

Where Q_{FF} and Q_{BB} are 2x2 matrices in advanced/retarded space whose components are Bosonic variables. Therefore, in order for the gaussian integral to converge, the diagonal components of Q_{BB} must be pure imaginary :

$$\mathrm{tr}\, Q^2 > 0 \Rightarrow \mathrm{tr}\, Q^2_{BB} < 0 \Rightarrow Q_{BB} = \begin{pmatrix} ib_{++} & -b_{+-} \\ b^*_{+-} & ib_{--} \end{pmatrix}, \tag{3.42}$$

where $b_{\pm\pm} \in \mathbb{R}$ such that $\mathrm{tr}\, Q^2_{BB} = -b^2_{++} - b^2_{--} - 2|b_{+-}|^2 < 0$. On the other hand, the Fermionic matrix $Q_{FF} = Q^\dagger_{FF}$ can be an arbitrary hermitian matrix, such that $\mathrm{tr}\, Q^2_{FF} = \lambda^2_{F,+} + \lambda^2_{F,-} > 0$, where $\lambda_{F,\pm} \in \mathbf{R}$ are the real eigenvalues of Q_{FF}. Now that the domain of Q is established (in accordance with condition (a)), the Hubbard-Stratonovich transformation for (3.39) gives :

$$e^{-\mathrm{tr}\,\frac{1}{4\pi\nu\tau}\sum_q A_{-\mathbf{q}}A_{\mathbf{q}}} = \int \mathcal{D}Q\, e^{-\mathrm{tr}\,\sum_q\left\{\frac{\pi\nu}{16\tau}Q_{-\mathbf{q}}Q_{\mathbf{q}} + \frac{i}{8\tau}(A_{-\mathbf{q}}Q_{\mathbf{q}} + Q_{-\mathbf{q}}A_{\mathbf{q}})\right\}}. \tag{3.43}$$

Bearing in mind that $\sum_{q \ll l^{-1}}$ restricts the external field to slowly variying modes $Q_{\mathbf{q}}$, we can rewrite (3.43) in real space as :

$$e^{-\frac{1}{4\pi\nu\tau}\sum_q A_{-\mathbf{q}}A_{\mathbf{q}}} = \int_{\text{slow modes}} \mathcal{D}Q\, e^{-\mathrm{tr}\int \mathrm{d}\mathbf{r}\left\{\frac{\pi\nu}{16\tau}Q^2 + \frac{i}{4\tau}\bar{\Psi}Q\Psi\right\}}, \tag{3.44}$$

where the restriction to slow variations of $Q(\mathbf{r})$ in the path integral will be implicitly assumed for the remainder of the report. Note that in supersymmetric case, $\mathcal{N} = 1$, and the normalization is unchanged by the HS transformation.

3.3.2 Integration of Supervector Fields and Wick's Theorem

Owing to the HS transformation, the effective action is now quadratic in Ψ with the cost of adding a new dynamic supermatrix field Q to the path integral :

$$\langle ... \rangle_{F[\Psi]} = \int \mathcal{D}\Psi \, e^{-F[\Psi]}(...) = \int \mathcal{D}Q \int \mathcal{D}\Psi \, e^{-F[\Psi;Q]}(...) =: \langle ... \rangle_{F[\Psi;Q]}, \tag{3.45}$$

where the new effective action $F[\Psi;Q]$ is given by :

$$F_\omega[\Psi;Q] = -\frac{1}{2}\mathrm{tr}\int \mathrm{d}\mathbf{r}\left(\bar{\Psi} g_\omega[Q]^{-1}\Psi + \frac{\pi\nu}{4\tau}Q^2\right) \tag{3.46}$$

$$g_\omega[Q]^{-1} := i\left(\hat{H}_{\omega^+} + \frac{\omega^+}{2}\Lambda + \frac{i}{2\tau}Q(\hat{\mathbf{r}})\right) \tag{3.47}$$

The SUSY approach started by showing the proportionality between conductivity $\sigma(\omega)$ and certain linear combinations of four-point functions of Ψ of the form $C_{IJKL}\langle \Psi^I(\mathbf{r})\bar{\Psi}^J(\mathbf{r})\Psi^K(0)\bar{\Psi}^L(0)\rangle_{F[Q]}$. Since $F_\omega[\Psi;Q] \propto \bar{\Psi} g_\omega[Q]^{-1}\Psi$, two-point functions in Ψ can be rewritten as Q-averages of Green's functions $g_\omega[Q](\mathbf{r},\mathbf{r}')$, namely :

$$\langle \Psi^I(\mathbf{r})\bar{\Psi}^J(\mathbf{r}')\rangle_{F_\omega[\Psi;Q]} = \langle g_\omega^{IJ}[Q](\mathbf{r},\mathbf{r}')\rangle_{F_\omega[Q]}, \tag{3.48}$$

where $F_\omega[Q]$ is the supervector-averaged action defined by :

$$e^{-F_\omega[Q]} := \int \mathcal{D}\Psi \, e^{-F_\omega[\Psi;Q]} = e^{-\frac{\pi\nu}{8\tau}\mathrm{tr}\int \mathrm{d}\mathbf{r}\, Q^2}\sqrt{\det g_\omega[Q]^{-1}}. \tag{3.49}$$

In (3.49), "det " is the superdeterminant, defined by $\det Q = \det Q_{FF}/\det Q_{BB}$ for $Q = Q_{FF} \oplus Q_{BB}$ in accordance with the formulae for scalar/Grassmannian gaussian integrals and the passage from supertrace to superdeterminant by exponentiation : $e^{\mathrm{tr}\,(...)} \equiv \det e^{(...)}$. Now, to write 4-point functions of Ψ in terms of $g_\omega[Q]$, we must use Wick's theorem :

$$\langle \Psi^I(\mathbf{r})\bar{\Psi}^J(0)\Psi^K(0)\bar{\Psi}^L(\mathbf{r})\rangle_{F_\omega[\Psi;Q]} = k_{JK}\langle g_\omega^{IL}(\mathbf{r},\mathbf{r})g_\omega^{KJ}(0,0)\rangle_{F_\omega[Q]} + \langle g_\omega^{IJ}(\mathbf{r},0)g_\omega^{KL}(0,\mathbf{r})\rangle_{F_\omega[Q]}, \tag{3.50}$$

In addition, since $Q(\hat{\mathbf{r}})$ in $g[Q]$ contains only the slowly varying modes $q \ll l^{-1}$, the propagator (3.47) should decay exponentially in real space over scales of the order of the mean free path, i.e. $g[Q](\mathbf{r},\mathbf{r}') \sim e^{-|\mathbf{r}-\mathbf{r}'|/l}$. This means that the product of $0 \leftrightarrow 0$, $\mathbf{r} \leftrightarrow \mathbf{r}$ propagators have a much larger contribution to (3.50) than the product of $0 \leftrightarrow \mathbf{r}$ propagators, such that :

$$\langle \Psi^I(\mathbf{r})\bar{\Psi}^J(0)\Psi^K(0)\bar{\Psi}^L(\mathbf{r})\rangle_{F_\omega[\Psi;Q]} \simeq k_{JK}\langle g_\omega^{IL}(\mathbf{r},\mathbf{r})g_\omega^{KJ}(0,0)\rangle_{F_\omega[Q]}. \tag{3.51}$$

3.3.3 Saddle Points of the Supermatrix Action

Now that all correlation functions in $\Psi\bar{\Psi}$ have been re-expressed Q-dependent quantities averaged over over the partition sum $e^{-F[Q]}$, we have translated the supervector field theory into a supermatrix field theory.

Saddle points $Q_T(\mathbf{r})$ of $F_\omega[Q]$ are defined by the vanishing of the functional differential $\delta F_\omega[Q_T] := 0$. Using $\delta \mathrm{tr}\, Q^2 = 2\mathrm{tr}\, Q\delta Q$ and $\delta \ln \mathcal{A}[Q] = \mathrm{tr}\, \mathcal{A}^{-1}[Q]\delta\mathcal{A}[Q]$ ("tr " can be seen here both as a supermatrix trace over I and a trace in position space over $\mathbf{r}$), we obtain :

$$4\tau\delta F_\omega[Q_T] = \mathrm{tr}\int \mathrm{d}\mathbf{r}\ \left(\pi\nu Q_T(\mathbf{r}) - g_\omega[Q_T](\mathbf{r},\mathbf{r})\right)\delta Q(\mathbf{r}) = 0 \iff Q_T(\mathbf{r}) = \frac{1}{\pi\nu}g_\omega[Q_T](\mathbf{r},\mathbf{r}). \tag{3.52}$$

Mean Field Saddle Points

In the case where $Q_T(\mathbf{r}) = \text{const}$, the saddle point equation (3.52) reduces to the mean field equation (3.24) for $Q \leftrightarrow \langle Q_\Psi\rangle$, with the AC solution $Q_T = \Lambda$ and the degenerate DC solutions $Q_T \in \mathcal{M}$. However, the constraints (3.42) on the Bosonic part of Q imply that it must have **imaginary** eigenvalues in the Bosonic sector, unlike $\Lambda_{BB} = \sigma_z^{\mathrm{AR}}$, which would imply that there is no mean field (translationally invariant) solution for Q! This problem can be solved by deforming the contour $\int \mathcal{D}Q_{BB}$ over the Bosonic sector of Q such that certain mean field solutions $Q = V\Lambda\bar{V}$ are well defined, albeit with an additional constraint on the supermatrices V (for a more detailed explanation, see [4], §4.2.2 or [5]) :

$$V^{-1} = \bar{V} \equiv KV^\dagger K, \tag{3.53}$$

where $K := \mathrm{diag}(1,1,1,-1) = \mathbb{1}^{\mathrm{FB}} \oplus \sigma_z^{\mathrm{FB}}$ is the supermatrix differing from Λ by $K_{--} = \sigma_z^{\mathrm{FB}} \neq -\mathbb{1}^{\mathrm{FB}}$. Therefore, as expected from the mean-field analysis, translationally-invariant solutions of the saddle point equation in the DC limit are given by arbitrary elements of the saddle point manifold, which is now explicitly as the orbit of Λ by the symmetry group G :

$$\mathcal{M} = \mathcal{O}_\Lambda := \left\{V\Lambda V^{-1}\right\}_{V\in G}, \tag{3.54}$$

where the symmetry group $G \subset G_\Psi$ obeys an extra constraint (c.f. (3.12)) :

$$G := \left\{ V \in G_\Psi \,|\, \bar{V} \equiv K V^\dagger K \right\}. \tag{3.55}$$

Arbitrary DC Saddle Points

In the DC limit $\omega \to 0$, the Green's function operator in the saddle point equation (3.52) is given by :

$$g_0[Q] \equiv g[Q] = i \left(\xi(\hat{\mathbf{p}}) + \frac{i}{2\tau} Q(\hat{\mathbf{r}}) \right)^{-1}. \tag{3.56}$$

As mentioned previously, general DC saddle points are expected to be given by arbitrary fluctuations on the manifold of mean field solutions, that is $Q(\mathbf{r}) = V(\mathbf{r})\Lambda\bar{V}(\mathbf{r}) \in \mathcal{M}$, $\forall \mathbf{r}$. This can be proven in the case of small fluctuations $Q(\mathbf{r}) \equiv Q_{MF} + \delta Q(\mathbf{r})$. In this case, we can make the expansion :

$$\begin{aligned} g[Q_{MF} + \delta Q] = \left(g[Q_{MF}]^{-1} + \frac{i}{\tau}\delta Q \right)^{-1} &= \left(\mathbb{1} + \frac{i}{\tau} g[Q_{MF}]\delta Q \right)^{-1} g[Q_{MF}] \\ &= g[Q_{MF}] - \frac{i}{\tau} g[Q_{MF}]\delta Q \, g[Q_{MF}] + \mathcal{O}(\delta Q^2). \end{aligned}$$

Since Q_{MF} automatically satisfies the saddle point equation, we can reduce (3.52) to :

$$\delta Q = \frac{1}{\pi\nu\tau} \langle \mathbf{r}| \, g[Q_{MF}]\delta Q \, g[Q_{MF}] \, |\mathbf{r}\rangle + \mathcal{O}(\delta Q^2). \tag{3.57}$$

We can now divide fluctuations δQ into two categories :

(T) : **Transverse** fluctuations or "**Goldsone** modes" $\delta_T Q$ are **tangent** to the saddle point manifold. its explicit form can be obtained by expanding an infinitesimal transformation $Q(\mathbf{r}) = V(\mathbf{r})Q_{MF}\bar{V}(\mathbf{r})$, where $V(\mathbf{r}) = e^{v(\mathbf{r})} = \mathbb{1} + v(\mathbf{r}) + \mathcal{O}(v^2)$ is continuously related to the identity, and $v \in \mathfrak{g}$ is in the Lie algebra of G. In this case the condition $V\bar{V} = V\Lambda V^\dagger \Lambda = \mathbb{1}$ for $V \in G$ translates to :

$$(1+v)\Lambda(1+v^\dagger)\Lambda = 1 + \mathcal{O}(v^2) \Rightarrow \bar{v} = \Lambda v^\dagger \Lambda = -v, \tag{3.58}$$

We can therefore parametrize $\delta_T Q$ in terms of v :

$$Q = e^{v} Q_{MF} e^{-v} = Q_{MF} + [v, Q_{MF}] + \mathcal{O}(v^2) \equiv Q_{MF} + \delta_T Q + \mathcal{O}(v^2), \tag{3.59}$$

which implies in particular :

$$\delta_T Q = (v + \bar{v}) Q_{MF} = -Q_{MF}(v + \bar{v}) \tag{3.60}$$

$$Q_{MF}\delta_T Q = -Q_{MF}^2(v + \bar{v}) = Q_{MF}(v + \bar{v})Q_{MF} = -\delta_T Q Q_{MF} \iff \{Q_{MF}, \delta_T Q\} = 0 \tag{3.61}$$

We can thus solve (3.57) using (3.61) :

$$\langle \mathbf{r}| \, g[Q_{MF}]\delta_T Q \, g[Q_{MF}] \, |\mathbf{r}\rangle = \langle \mathbf{r}| \, g[Q_{MF}] g[-Q_{MF}] \, |\mathbf{r}\rangle \, \delta_T Q(\mathbf{r}). \tag{3.62}$$

Using $Q_{MF}^2 = \Lambda^2 = \mathbb{1}$, (3.62) greatly simplifies :

$$g[Q_{MF}]g[-Q_{MF}] = -\left[\left(\xi(\hat{\mathbf{p}}) - \frac{i}{2\tau} Q_{MF}\right)\left(\xi(\hat{\mathbf{p}}) + \frac{i}{2\tau} Q_{MF}\right)\right]^{-1} = -\left(\xi(\hat{\mathbf{p}}) + (2\tau)^{-2}\right)^{-1} \mathbb{1}. \tag{3.63}$$

We can then directly compute the $(\mathbf{r}, \mathbf{r})$ component of (3.63) as a momentum integral :

$$\begin{aligned} \langle \mathbf{r}| \, g[Q_{MF}] g[-Q_{MF}] \, |\mathbf{r}\rangle &= \int \frac{\mathrm{d}^d \mathbf{p}}{(2\pi)^d} \frac{1}{\xi(\mathbf{p})^2 + (\tau/2)^{-2}} \\ &\simeq \nu \int_{\mathbb{R}} \mathrm{d}\xi \, \frac{1}{\xi^2 + (2\tau)^{-2}} = \pi\nu\tau \end{aligned}$$

With a similar analysis up to arbitrary orders $\mathcal{O}(\delta_T Q^n)$, we can show that the saddle point equation (3.52) is automatically satisfied for transverse fluctuations $Q_T(\mathbf{r}) := V(\mathbf{r})\Lambda\bar{V}(\mathbf{r})$ on the saddle point manifold, where $V(\mathbf{r})$ is continuously related to the identity. However, it is important to note that the perturbative saddle point equation (at arbitrary order) neglects solutions $\mathbf{r} \to Q(\mathbf{r}) \in \mathcal{M}$ where $\{Q(\mathbf{r})\}_{\mathbf{r}}$ covers several time the whole manifold. These modes cannot be continuously parametrized in terms of local coordinates on $\mathcal{M}$, and can play an important role in topological transport phenomena.

(L) **Longitudinal** or "**massive**" fluctuations are defined by variations in directions **perpendicular** to the manifold in Q-space. This corresponds to variations of the **eigenvalues** of $Q_{MF} = V\Lambda V^{-1} \in \mathcal{M}$, and can be parametrized by : $Q(\mathbf{r}) = V(\Lambda + \delta\Lambda(\mathbf{r}))\bar{V}$, where $\delta\Lambda(\mathbf{r}) := \mathrm{diag}(\delta\lambda^I(\mathbf{r}))_{I=(F/B,\pm)}$. The above parametrization $\delta_L Q(\mathbf{r}) := V\delta\Lambda(\mathbf{r})\bar{V}$ is equivalent to imposing :

$$[Q_{MF}, \delta_L Q] = V\,[\Lambda, \delta\Lambda]\,\bar{V} = 0. \tag{3.64}$$

This implies that we can rewrite (3.57) as :

$$\langle \mathbf{r}|\, g[Q_{MF}]\delta_L Q\, g[Q_{MF}]\,|\mathbf{r}\rangle = \langle \mathbf{r}|\, g[Q_{MF}]g[+Q_{MF}]\,|\mathbf{r}\rangle\, \delta_L Q(\mathbf{r}). \tag{3.65}$$

However, we have in this case $g[Q_{MF}]^2 = V\left(\xi(\hat{\mathbf{p}}) + \frac{i}{2\tau}\Lambda\right)^{-2}\bar{V}$, which leads to a vanishing momentum integral :

$$\begin{aligned}\langle \mathbf{r}|\, g[Q_{MF}]^2_{IJ}\,|\mathbf{r}\rangle &= V_{IK}\int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi)^d}\left(\frac{1}{\xi(\mathbf{p}) + i\Lambda_{II}(2\tau)^{-1}}\right)^2 \bar{V}_{KJ} \\ &\simeq \nu\, V_{IK}\int_{\mathbb{R}} \mathrm{d}\xi\,\left(\frac{1}{\xi + i\Lambda_{II}(2\tau)^{-1}}\right)^2 \bar{V}_{KJ} = 0\end{aligned}$$

Therefore, only the trivial solution $\delta_L Q = 0$ satisfies the infinitesimal saddle point equation (3.57) for longitudinal fluctuations, i.e. massive fluctuations leave the saddle point manifold.

3.4 From the Supermatrix Action to a NLSM on the Saddle Point Manifold

Since diagonal elements of the Green's function correspond to saddle points according to (3.52), we can rewrite the Q-averages (3.51) as 2-point functions of saddle points $Q_T(\mathbf{r}) = V(\mathbf{r})\Lambda\bar{V}(\mathbf{r})$, meaning that only fluctuations on the saddle point manifold contribute to conductivity :

$$\sigma(\omega) \propto \mathbb{E}[G^A_{\epsilon-\omega}(\mathbf{r},0)G^R_\epsilon(0,\mathbf{r})] \simeq C_{IJKL}\langle Q_T^{IJ}(\mathbf{r})Q_T^{KL}(0)\rangle_{F[Q]}. \tag{3.66}$$

Knowing this, we can reduce $F[Q]$ to a field theory on $\mathcal{M} \ni Q_T$ following the procedure below :

1. find the appropriate DC limit $F_{\omega\to 0}[Q]$,
2. decompose the path integral into longitudinal/transverse contributions by expanding the action $F[Q_{MF} + \delta_T Q + \delta_L Q]$ around a mean field saddle point,

3. and integrate out the longitudinal modes in the path integral to obtain an action describing a non-linear sigma model (NLσM) on the saddle point manifold $\mathcal{M}$.

3.4.1 Linearization of the $\omega\Lambda$-contribution

As mentioned previously, the $\omega\Lambda$-term, which is now in $\ln g_\omega[Q]^{-1}$ breaks the V-symmetry similarly to a weak external field. In the DC limit $\omega^+ \to i0^+$, we can expand $\mathrm{tr}\,\ln g_\omega[Q]^{-1}$ to obtain once again a linear contribution :

$$\begin{aligned} F_\omega[Q] &= F_0[Q] + \frac{dF_{\omega=0}[Q]}{d\omega}\,\omega^+ + \mathcal{O}(\omega^2) \\ &= F_0[Q] - \frac{i\omega}{2\pi\nu\tau}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,\Lambda Q + \mathcal{O}(\omega^2), \end{aligned}$$

using $\frac{d}{d\omega}\mathrm{tr}\,f(A(\omega)) = \mathrm{tr}\,f'(A(\omega))\frac{dA}{d\omega}$. The zero-frequency action is now given by :

$$F_0[Q] = \mathrm{tr}\int \mathrm{d}\mathbf{r}\,\left(\frac{\pi\nu}{8\tau}Q^2 - \frac{1}{2}\ln g[Q]^{-1}\right), \tag{3.67}$$

where $g[Q] = i\left(\xi(\hat{\mathbf{p}}) + \frac{i}{2\tau}\Lambda\right)^{-1}$.

3.4.2 Gaussian Expansion in $F[Q]$

We now consider arbitrary fluctuations $Q(\mathbf{r}) \equiv Q_{MF} + \delta Q(\mathbf{r})$ around a mean-field saddle point Q_{MF}. In the limit of small fluctuations $\delta Q \ll 1$, we can approximate $F_0[Q_{MF} + \delta Q]$ by its leading order fluctuations, which corresponds to a Gaussian expansion around Q_{MF}

$$F_0[Q_{MF} + \delta_t Q] = F_0[Q_{MF}] + \delta F_0[Q] + \frac{1}{2}\delta^2 F_0[Q] + \mathcal{O}(\delta Q^3), \tag{3.68}$$

where $\delta^2 F_0[Q] = \mathrm{tr}\int \mathrm{d}\mathbf{r}\int \mathrm{d}\mathbf{r}'\,\delta Q(\mathbf{r})\frac{\delta^2 F_0[Q_{MF}]}{\delta Q(\mathbf{r})\delta Q(\mathbf{r}'))}\delta Q(\mathbf{r}')$. As in the mean-field case, we have $F_0[Q_{MF}] \propto \mathrm{tr}\,\Lambda, \mathrm{tr}\,\mathbb{1} = 0$ since $\mathrm{tr}\,VAV = \mathrm{tr}\,A$. The second variation $\delta^2 F_0$ of (3.67) will behave very differently depending on whether $\delta_X Q$ is transverse ($X = T$) or longitudinal ($X = L$) :

- The Gaussian expansion of the quadratic part of (3.67) is given by : $\delta_X^2 \int \mathrm{d}\mathbf{r}\,Q(\mathbf{r})^2 =$

$2\int \mathrm{d}\mathbf{r}\, \delta_X Q(\mathbf{r})^2$.

- The variation of the logarithmic part of (3.67) is given by :

$$\begin{aligned}\delta^2 \int \mathrm{d}\mathbf{r}\, \mathrm{tr}\, \ln g[Q](\mathbf{r}) &= \frac{1}{2\tau}\delta\left(\int \mathrm{d}\mathbf{r}\, \mathrm{tr}\, g[Q](\mathbf{r},\mathbf{r})\delta Q(\mathbf{r})\right) \\ &= \frac{1}{4\tau^2}\int \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{r}'\, \mathrm{tr}\, g[Q](\mathbf{r},\mathbf{r}')\delta Q(\mathbf{r}')g[Q](\mathbf{r}',\mathbf{r})\delta Q(\mathbf{r})\end{aligned}$$

and as a consequence of (3.61), (3.64) :

$$g[Q](\mathbf{r},\mathbf{r}')\delta_X Q = \delta_X Q g[(-)^X Q](\mathbf{r},\mathbf{r}'), \tag{3.69}$$

where $(-)^L = +1$ and $(-)^T = -1$ distinguishes the commutation properties of longitudinal and transverse fluctuations with the mean field saddle point Q (see Sec. 3.3.3).

The Gaussian expansion for transverse/longitudinal modes is thus given by :

$$F_0[Q_{MF}+\delta_X Q] = \frac{\pi\nu}{8\tau}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,(\delta_X Q)^2 - \frac{1}{2\tau^2}\mathrm{tr}\int \mathrm{d}\mathbf{r}\left\{\int \mathrm{d}\mathbf{r}'\, g[Q](\mathbf{r},\mathbf{r}')g[(-)^X Q](\mathbf{r}',\mathbf{r})\right\}\delta_X Q(\mathbf{r}')\delta_X Q(\mathbf{r}). \tag{3.70}$$

3.4.3 Gradient Expansion of The Quadratic Action

Since $g[Q](\mathbf{r},\mathbf{r}') \sim e^{|\mathbf{r}-\mathbf{r}'|/l}$ falls off like the mean free path, we can spatially expand both fluctuations $\delta_X Q(\mathbf{r}/\mathbf{r}')$ in (3.70) :

$$\delta_X Q(\mathbf{x} \pm \mathbf{y}/2) = \delta_X Q(\mathbf{x}) \pm \frac{1}{2}\mathbf{y}\cdot\boldsymbol{\nabla}\delta_X Q(\mathbf{x}) + \mathcal{O}(l^2), \tag{3.71}$$

where $\mathbf{r} := \mathbf{x} + \mathbf{y}/2$ and $\mathbf{r}' := \mathbf{x} - \mathbf{y}/2$ is a convenient variable change such that $\mathbf{r} - \mathbf{r}' = \mathbf{y} = \mathcal{O}(l)$.

- At order $\mathcal{O}(l^0)$:

$$\begin{aligned}\int \mathrm{d}\mathbf{y} \quad & g_0[Q](\mathbf{x}-\mathbf{y}/2,\mathbf{x}+\mathbf{y}/2)g_0[(-)^X Q](\mathbf{x}+\mathbf{y}/2,\mathbf{x}-\mathbf{y}/2)\\ = \quad & \int \mathrm{d}\mathbf{r}'\, g_0[Q](\mathbf{r},\mathbf{r}')g_0[-Q](\mathbf{r}',\mathbf{r})\\ = \quad & \langle\mathbf{r}|\, g[Q]g[(-)^X Q]\,|\mathbf{r}'\rangle\\ = \quad & -\pi\nu\tau\delta_{XT},\end{aligned}$$

  according to (3.62) and (3.65).

  This provides a term quadratic in $\delta_T Q(\mathbf{r})$ that cancels with the transverse variation of the quadratic term $\frac{\pi\nu}{8\tau}\int \mathrm{d}\mathbf{r}\,\mathrm{tr}\,\delta_T Q(\mathbf{r})^2$.

- At order $\mathcal{O}(l)$, we expect the integral to cancel in an isotropic material, since $g[Q](\mathbf{r},\mathbf{r}') \equiv g[Q](|\mathbf{r}-\mathbf{r}'|)$ should not depend on the direction of $\mathbf{r}-\mathbf{r}'$:

$$\int \mathrm{d}\mathbf{y}\ \mathbf{y}\, g[Q](\mathbf{x}-\mathbf{y}/2,\mathbf{x}+\mathbf{y}/2)g[-Q](\mathbf{x}+\mathbf{y}/2,\mathbf{x}-\mathbf{y}/2) \equiv 0.$$

- At order $\mathcal{O}(l^2)$, isotropy now limits the form of the integral to :

$$\int \mathrm{d}\mathbf{y}\ y_i y_j\, f(|\mathbf{y}|) \equiv \frac{\delta_{ij}}{d}\int \mathrm{d}\mathbf{y}\ \mathbf{y}^2\, f(|\mathbf{y}|). \tag{3.72}$$

  We can make the further approximation :

$$\int \mathrm{d}\mathbf{y}\ \mathbf{y}^2\, f(|\mathbf{y}|) \simeq l^2 \int \mathrm{d}\mathbf{y}\, f(|\mathbf{y}|) = -l^2\pi\nu\tau\delta_{XT}, \tag{3.73}$$

  with $f(|\mathbf{y}|) = g[Q](\mathbf{r},\mathbf{r}')g[(-)^X Q](\mathbf{r}',\mathbf{r}) \sim e^{-|\mathbf{y}|/l}$ decays sufficiently fast for variations in $\mathbf{y}^2$ to be negligeable in (3.73).

Longitudinal Fluctuations

Up to order $\mathcal{O}(l^2)$ in the gradient expansion, the only contribution to longitudinal fluctuations in the Gaussian approximation comes from the quadratic (mass) term in (3.67), hence the term "massive fluctuations" :

$$F_0[Q_{MF}+\delta_L Q] = \frac{\pi\nu}{8\tau}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,\delta_L Q^2 + \mathcal{O}(\delta_L Q^3; l^3). \tag{3.74}$$

As shown previously, we are only interested in correlation functions of supermatrices on the saddle point manifold, so we can integrate out all fluctuations $\delta_L Q$ that leave the saddle point manifold in the path integral. From (3.74), this corresponds to a supersymmetry Gaussian integral, which therefore leaves no normalization factor to the remaining partition function :

$$\int \mathcal{D}\delta_L Q\, e^{-F_0[Q_{MF}+\delta_L Q]} = \int \mathcal{D}\delta_L Q\, e^{-\frac{\pi\nu}{8\tau}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,\delta_L Q^2} = 1. \tag{3.75}$$

Transverse Fluctuations

As mentioned before, the $\mathcal{O}(l^0)$-term in the gradient expansion of the logarithmic term cancels out with the transverse variation of the quadratic term in (3.67) so that transverse modes are effectively "massless". Therefore, the only remaining term lower than order l^2 is the kinetic term :

$$F_0[Q_{MF}+\delta_T Q] = \frac{\pi\nu l^2}{8\tau d}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,|\boldsymbol{\nabla}\delta_T Q(\mathbf{r})|^2 + \mathcal{O}(\delta_T Q^3; l^3). \tag{3.76}$$

3.4.4 Non Linear Sigma Model

After integrating out the longitudinal modes in (3.75), the resulting field theory is defined solely on the saddle point manifold $Q_T(\mathbf{r}) = Q_{MF} + \delta_T Q(\mathbf{r}) = V(\mathbf{r})\Lambda\bar{V}(\mathbf{r}) \in \mathcal{M}$:

$$\int \mathcal{D}Q\, e^{-F[Q]} = \int \mathcal{D}\delta Q_T\, e^{-F_\omega[Q_{MF}+\delta Q_T]} =: \int \mathcal{D}Q_T\, e^{-F_\omega[Q_T]}. \tag{3.77}$$

If we define the diffusion coefficient $D_0 := \frac{l^2}{\tau d} = v_F^2\tau/d$, the effective action describing the Goldstone modes on $\mathcal{M}$ is given by :

$$F_\omega[Q_T] = \frac{\pi\nu}{8}\mathrm{tr}\int \mathrm{d}\mathbf{r}\,\left\{D_0(\boldsymbol{\nabla}Q_T)^2 + i2\omega^+\Lambda Q_T\right\}. \tag{3.78}$$

The effective field theory (3.78) is called a (supermatrix) **non linear sigma model**. Note that the non-linearity here comes only from the fact that the supermatrix field is defined on a manifold that is not generally flat. In the DC limit, this model contains only one coupling constant $t^{-1} := \pi\nu D_0/8$, whose renormalization provides all the information on the conductivity of the metallic system. This, in turn, depends crucially on the properties of the

manifold $\mathcal{M}$ (or alternatively the symmetry group G) on which the NLSM is defined. The limits of this model lie essentially in the validity of the Gaussian approximation (3.68) for the (exact) action in (3.49). Unlike the gradient expansion of Sec. 3.4.3, there is no small parameter that can be constructed from the physical inputs ν,τ,l to justify the perturbative expansion. In particular, topologically non-trivial modes can contribute to the path integral with additional topological terms in (3.78) that evade perturbation theory, leading to topological transport phenomena such as the Integer Quantum Hall Effect. As such, the NLσM should be used with caution beyond the perturbative Cooperon/Diffuson-dominated regime.

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