

Lecture Notes: Introduction to Condensed Matter Theory

Titus Neupert¹

¹*Department of Physics, University of Zurich,
Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*

(Dated: June 1, 2017)

CONTENTS

Plan of the lectures	4
I. Introduction	4
II. From quantum statistical mechanics to condensed matter	7
A. Basic concepts	7
1. Second quantization	7
2. Hamiltonians and partition functions	10
3. Thermodynamic potentials	13
4. Spontaneous symmetry breaking	14
5. Mean-field approximation	17
B. Linear response	18
C. Symmetries in condensed matter	20
1. Non-local vs. local, unitary vs. antiunitary	20
2. Symmetries of a crystal	21
3. Reciprocal space	23
III. Noninteracting electron systems	25
A. Bloch's theorem	25
B. Nearly free electron approximation	26
C. Tight-binding approximation	28
D. Wannier states	31
E. Interlude: Group representations and character tables	32
F. Symmetries in band structures	35
G. Filling of bands and density of states	37
H. Coupling to an external electro-magnetic field	38
1. Semiclassical equations of motion	39
2. The integer quantum Hall effect	41
3. Quantum oscillations	46
I. Phonons	49
1. Quantizing lattice vibrations	49

2. Peierls instability in 1D	51
IV. Interactions in itinerant systems	54
A. Particle-hole excitations	54
1. In semiconductors	54
2. In metals	57
B. Fermi liquid theory	62
1. Quasiparticles	62
2. Basics of Landau Fermi liquids	64
3. Compressibility and susceptibility	66
C. Transport in metals	67
1. Linear response and complex analysis	67
2. Boltzmann transport theory	69
3. Conductivity	70
4. Optical properties	72
5. Computing the relaxation time	73
D. Interacting instabilities	76
1. The fractional quantum Hall effect	76
2. Superconductivity	78
3. Density waves	84
4. Mott insulators	87
V. Magnetism in solids	92
A. Antiferromagnetism	92
1. Superexchange in the Hubbard model	92
2. Mean-field theory and its shortcomings	94
3. Spin-wave theory	96
B. Stoner magnetism	100
1. Mean-field theory	101
2. Susceptibility on the paramagnetic side	104
3. Magnons	105

PLAN OF THE LECTURES

1. 23. Feb: I. Intro; II. Basic concepts
2. 2. Mar: DOUBLE LECTURE II. Linear response, III. Symmetries, Reciprocal space, Bloch's theorem
3. 9. Mar: III. Tight-binding, nearly free electron
4. 16. Mar: NO LECTURE
5. 23. Mar: Band structure theory
6. 30. Mar: III. Electrons in a magnetic field
7. 6. Apr: Phonons in metals, Peierls instability
8. 13. Apr: IV. Semiconductors vs. metals: Charged excitations
9. 27. Apr: IV. Fermi liquid theory, transport in metals
10. 4. May: IV. Fractional quantum Hall effect and superconductivity
11. 11. May: IV. Density waves and Mott insulators
12. 18. May: V. Antiferromagnetism
13. 1. Jun: V./IV. Stoner magnetism and numerical tools

I. INTRODUCTION

The study of quantum condensed matter is a very hard problem. We consider in general interacting many-body systems of 10^{24} degrees of freedom, typically represented by the electrons in a solid. Since the Hilbert space is exponentially large in the number of degrees of freedom, any 'brute force' theoretical approach using the resources of classical computers to this problem must fail. A quantum computer might help, but is not (yet) available. Nevertheless, impressive progress has been made in the theoretical study of solid state systems, thanks to two bold simplifications:

Separation of energy scales: In contrast to high-energy physics, where new physics appears at ever higher energies, in condensed matter physics the phenomena of interest typically appear at very low energies. To put it boldly, these two energy frontiers are where we can expect new physics to appear. Everything in between is, at least on a fundamental level, understood. Different physical phenomena can be separated by the energy scale at which they appear, and their impact on the phenomena at smaller energy scales can often be incorporated in some effective form. For example, it is in many cases sufficient to consider the crystal as a rigid lattice of ions in which the electrons move or to only consider the coupling between the electrons and the low-energy vibration (phonon) modes of the crystal. As another example, the Coulomb interaction between electrons can in some cases be neglected so that one solves only the problem of free electrons moving in the background potential of the ions. A plethora of more sophisticated approximations has been developed, some of which we will encounter in this course.

Use of symmetries: The formation of a crystal breaks (spontaneously) the Lorentz symmetry of open space. At first sight, this appears to be problematic, as one cannot take advantage of this symmetry group to describe the low-energy properties of electrons, in the same way as one can identify allowed terms in a Lagrangian in high-energy physics, say. However, the crystal breaks the symmetry not completely, but retains a discrete translation symmetry and potentially other symmetries such as rotations, mirror reflections, inversion, time-reversal symmetry and so on. In addition, at low energies effective symmetries can emerge that are not shared by the whole crystal. For example, while a cubic crystal has only four-fold rotational symmetry, the dispersion of electrons at low electron-density might still be well described as parabolic, with an effective continuous rotation symmetry. This renders the situation much better than, say, in bio-chemistry, where one cannot take much advantage of constraining the problems by symmetries.

Thus, the 'master equation' for solid state systems in equilibrium is given by the Hamil-

tonian

$$\begin{aligned}
H &= H_{0,e} + H_{0,i} + H_{e-e} + H_{i-i} + H_{i-e}, \\
H_{0,e} &= \sum_j (\boldsymbol{\alpha} \cdot \mathbf{p}_j + \beta m_e), \\
H_{0,i} &= \sum_j \frac{\mathbf{P}_j^2}{2M_j}, \\
H_{e-e} &= \sum_{j,l} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_l|}, \quad H_{e-i} = \sum_{j,l} \frac{e^2 Z_l}{|\mathbf{r}_j - \mathbf{R}_l|}, \quad H_{i-i} = \sum_{j,l} \frac{e^2 Z_j Z_l}{|\mathbf{R}_j - \mathbf{R}_l|},
\end{aligned} \tag{1}$$

where \mathbf{p}_j and \mathbf{r}_j are momentum and position operator of the j -th electron, m_e is the electron mass, \mathbf{P}_j and \mathbf{R}_j are momentum and position operator of the j -th nucleus, Z_j and M_j are its charge and mass. The Dirac form of the electronic kinetic Hamiltonian was chosen to include the physics of spin-orbit coupling, which is important to topics of recent interest in solid state physics. Hamiltonian (1) is essentially impossible to solve without further approximations. (What is not included in Hamiltonian (1) is the physics associated with the nuclear spins.)

To make progress in understanding a specific phenomenon or system, one often works with a toy model. While such models can be motivated using qualitative or quantitative arguments, solid state theorists can become very creative in dreaming up new models. Sometimes, these models are still very hard to solve, like the paradigmatic Hubbard model, for example. In other cases, the advantage of a specific model might be its exact solubility, as is the case with the transverse-field Ising model, for example.

- general trends in the periodic table of elements: masses, sizes, spin-orbit coupling

Equilibrium vs. non-equilibrium properties

II. FROM QUANTUM STATISTICAL MECHANICS TO CONDENSED MATTER

A. Basic concepts

1. Second quantization

In first quantization, we denote the (non-degenerate) quantum state of a many-body system of N identical particles by a wave function

$$\Psi(\alpha_1, \alpha_2, \dots, \alpha_N), \quad (2)$$

where the α_i , $i = 1, \dots, N$ run over labels for a basis of the single-particle Hilbert space \mathcal{H}_1 and each α_i denotes the single-particle state that the i -th particle is in. For example, α could label the position of a particle and in addition some internal degrees of freedom such as spin. The Pauli principle, the axiom underlying many-body quantum mechanics, says that equivalent particles are indistinguishable. Any observables, such as the probability density, may thus not depend on the order in which the states α_i of indistinguishable particles are listed in the arguments of Ψ . For the exchange of only two particles, this amounts to impose the equality

$$|\Psi(\alpha_1, \dots, \alpha_i, \dots, \alpha_j, \dots, \alpha_N)|^2 = |\Psi(\alpha_1, \dots, \alpha_j, \dots, \alpha_i, \dots, \alpha_N)|^2. \quad (3)$$

Thus, upon exchange, Ψ could be multiplied by an arbitrary phase $e^{i\varphi(\alpha_i, \alpha_j)}$. However, exchanging the particles twice needs to bring the wave function back to itself, in order for the wave function to be single valued, i.e., $e^{i\varphi(\alpha_i, \alpha_j)} = \pm 1$. (Non-degenerate wave functions that are not single-valued are not permitted.) As a result, there are only two possibilities

$$\Psi(\alpha_1, \dots, \alpha_i, \dots, \alpha_j, \dots, \alpha_N) = \pm \Psi(\alpha_1, \dots, \alpha_j, \dots, \alpha_i, \dots, \alpha_N), \quad (4)$$

which correspond to bosons (the $+$ sign) and fermions (the $-$ sign).

We recall that the N -particle Hilbert space \mathcal{H}_N is a direct product of N copies of the single-particle Hilbert space, and the Fock space \mathcal{F} is a direct sum over these

$$\mathcal{H}_N := \bigotimes_{i=1}^N \mathcal{H}_1, \quad \mathcal{F} := \bigoplus_{N=1}^{\infty} \mathcal{H}_N, \quad (5)$$

where \mathcal{H}_0 is a one-dimensional space spanned by the vacuum $|0\rangle$ alone. A basis for the N -particle Hilbert space is then given by

$$\Psi(\alpha_1, \alpha_2, \dots, \alpha_N) = \frac{1}{\sqrt{N!}} \sum_{p \in P_N} (\pm 1)^{\sigma(p)} \psi_{\alpha_1}(p_1) \psi_{\alpha_2}(p_2) \cdots \psi_{\alpha_N}(p_N), \quad (6)$$

where the sum runs over all permutations p of the first N integers, $\sigma(p)$ denotes the sign of the permutation, and the signs $(+1)$ and (-1) apply to bosons and fermions, respectively. Here, ψ_α are a set of basis functions of the single-particle Hilbert space \mathcal{H} . The basis functions (6) of \mathcal{H}_N are thus fully symmetrized (antisymmetrized) products of N single-particle basis functions ψ_α in the case of bosons (fermions). The latter can be written in the form of a determinant of the matrix with elements $M_{ij} = \psi_{\alpha_i}(j)$, $i, j = 1, \dots, N$, the so-called Slater determinant. In bra-ket notation, the state corresponding to Eq. (6) is often written in the *occupation number representation* by listing the number of particles that are occupying a each single particle state α by n_α . For fermions, $n_\alpha = 0, 1$, for the fully antisymmetric wave function (6) vanishes if two or more particles occupy the same single-particle state. For bosons, n_α can be any nonnegative integer. For example, in a system with a five-dimensional single-particle Hilbert space \mathcal{H}_1 (i.e., in which α can only take 5 different values), we would denote the state with 3 particles, that occupy the first, third, and forth single particle state by

$$\Psi(1, 3, 4) \quad \text{or} \quad |\{n_\alpha\}\rangle = |1, 0, 1, 1, 0\rangle. \quad (7)$$

The key object of the second-quantized formalism are particle creation operators \hat{c}_α^\dagger and annihilation operators \hat{c}_α . For fermions, these operators act as

$$\begin{aligned} \hat{c}_\alpha^\dagger |n_1, \dots, n_\alpha, \dots\rangle &= \delta_{n_\alpha, 0} (-1)^{n_1 + \dots + n_{\alpha-1}} |n_1, \dots, n_\alpha + 1, \dots\rangle, \\ \hat{c}_\alpha |n_1, \dots, n_\alpha, \dots\rangle &= \delta_{n_\alpha, 1} (-1)^{n_1 + \dots + n_{\alpha-1}} |n_1, \dots, n_\alpha - 1, \dots\rangle, \end{aligned} \quad (8)$$

and obey the relations

$$\{\hat{c}_\alpha, \hat{c}_{\alpha'}^\dagger\} = \delta_{\alpha, \alpha'}, \quad \{\hat{c}_\alpha, \hat{c}_{\alpha'}\} = \{\hat{c}_\alpha^\dagger, \hat{c}_{\alpha'}^\dagger\} = 0, \quad (9)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is the anticommutator. For bosons, they act as

$$\begin{aligned} \hat{c}_\alpha^\dagger |n_1, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha + 1} |n_1, \dots, n_\alpha + 1, \dots\rangle, \\ \hat{c}_\alpha |n_1, \dots, n_\alpha, \dots\rangle &= \sqrt{n_\alpha} |n_1, \dots, n_\alpha - 1, \dots\rangle, \end{aligned} \quad (10)$$

and obey the relations

$$[\hat{c}_\alpha, \hat{c}_{\alpha'}^\dagger] = \delta_{\alpha, \alpha'}, \quad [\hat{c}_\alpha, \hat{c}_{\alpha'}] = [\hat{c}_\alpha^\dagger, \hat{c}_{\alpha'}^\dagger] = 0. \quad (11)$$

For example, the occupation number of a state α can be measured with the operator $\hat{c}_\alpha^\dagger \hat{c}_\alpha$, because $\hat{c}_\alpha^\dagger \hat{c}_\alpha |n_1, \dots, n_\alpha, \dots\rangle = n_\alpha |n_1, \dots, n_\alpha, \dots\rangle$. Any state in the basis of \mathcal{F} can be generated by application of a product of \hat{c}_α^\dagger operators to the vacuum state $|0\rangle$, i.e.,

$$|\{n_\alpha\}\rangle = \prod_\alpha (\hat{c}_\alpha^\dagger)^{n_\alpha} |0\rangle, \quad (12)$$

where it is understood that $(\hat{c}_\alpha^\dagger)^0$ is the identity.

The second quantized operators transform natural under a basis change of the single particle Hilbert space \mathcal{H}_1 . Let $u_{\alpha,a} = \langle \alpha | a \rangle$ be the matrix elements of the unitary operator that encodes the change from a basis ψ_α of \mathcal{H}_1 to a different basis ψ_a . Then,

$$\hat{c}_a^\dagger = \sum_\alpha u_{\alpha,a} \hat{c}_\alpha^\dagger, \quad \hat{c}_a = \sum_\alpha u_{\alpha,a}^* \hat{c}_\alpha. \quad (13)$$

This transformation also applies if the label a is a continuous variable, such as the position \mathbf{r} of a particle, in which case we obtain the field operators

$$\hat{\phi}^\dagger(\mathbf{r}) = \sum_\alpha \langle \alpha | \mathbf{r} \rangle \hat{c}_\alpha^\dagger, \quad \hat{\phi}(\mathbf{r}) = \sum_\alpha \langle \mathbf{r} | \alpha \rangle \hat{c}_\alpha \quad (14)$$

that obey in the case of fermions

$$\{\hat{\phi}(\mathbf{r}), \hat{\phi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}'), \quad \{\hat{\phi}(\mathbf{r}), \hat{\phi}(\mathbf{r}')\} = \{\hat{\phi}^\dagger(\mathbf{r}), \hat{\phi}^\dagger(\mathbf{r}')\} = 0, \quad (15)$$

and in the case of bosons

$$[\hat{\phi}(\mathbf{r}), \hat{\phi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), \quad [\hat{\phi}(\mathbf{r}), \hat{\phi}(\mathbf{r}')] = [\hat{\phi}^\dagger(\mathbf{r}), \hat{\phi}^\dagger(\mathbf{r}')] = 0. \quad (16)$$

For example, a transformation of the form (14) is relevant to the case of a particle on a ring of circumference L , i.e., $r \in [0, L)$ with periodic boundary conditions. The momentum k takes discrete values $k = 2\pi l/L$, $l \in \mathbb{Z}$ (like the index α), while r is continuous. The coefficients $\langle k | r \rangle$ are nothing but the Fourier modes and we get

$$\hat{\phi}^\dagger(r) = \frac{1}{\sqrt{L}} \sum_k e^{ikr} \hat{c}_k^\dagger, \quad (17)$$

with the sum running over $k = 2\pi l/L$, $l \in \mathbb{Z}$, as the transformation law between the operator \hat{c}_k^\dagger that creates a particle with momentum k on the ring and the operator $\hat{\phi}^\dagger(r)$ that creates a particle at position r on the ring.

2. Hamiltonians and partition functions

Most of the time, we are interested in the properties of the unperturbed condensed matter system, or in its repose to small perturbations. In the former case, we can treat the system as closed, neither exchanging energy nor particles with the environment (corresponding to the microcanonical ensemble of statistical mechanics). In the latter case, we can use the isolated system as a good starting point for perturbative calculations within linear response theory.

Within the Hamiltonian formalism, the energy conserving system is described by a Hamiltonian \hat{H} that acts on the Hilbert or Fock space. Finding the eigenvalues and eigenstates of this operator amounts to solving the problem, a task that is often too hard to be achieved without further approximations. The Hamiltonian can be given either in first or second quantization. For the free particle of mass m on the ring with periodic boundary conditions, its first quantized version is

$$\hat{H}_\mu = \frac{\hat{p}^2}{2m} - \mu, \quad (18)$$

where \hat{p} is the momentum operator that has the representation $\hat{p} = -i\frac{d}{dr}$ in the position basis of the single particle Hilbert space. (Throughout these notes, we will set $\hbar = 1$, and only reinstate it in specific places to connect to well known-results in the right units.) The real number μ is the chemical potential the meaning of which will be discussed below. In the second quantized formulation, we can express H_μ either in the operators $\hat{\phi}(r)$ or \hat{c}_k

$$\hat{H}_\mu = \int_0^L dr \hat{\phi}^\dagger(r) \left(-\frac{1}{2m} \frac{d^2}{dr^2} - \mu \right) \hat{\phi}(r) = \sum_k \left(\frac{k^2}{2m} - \mu \right) \hat{c}_k^\dagger \hat{c}_k, \quad (19)$$

where we used that

$$\int_0^L \frac{dr}{L} e^{i(k-k')r} = \delta_{k,k'}. \quad (20)$$

Notice that the term multiplying μ is nothing but the operator $\hat{N} := \sum_k \hat{c}_k^\dagger \hat{c}_k$ that counts the total number of particles in the system. From Eq. (19) we see that we have diagonalized the Hamiltonian in momentum space, and its eigenvalues when acting on the single-particle Hilbert space \mathcal{H}_1 are the energy levels of the system, given by $\varepsilon_k = k^2/(2m) - \mu$, with $k = 2\pi l/L$, $l \in \mathbb{Z}$. The $2\pi/L$ discretization is due to the finite size of the system. One frequently encounters this splitting when considering small systems that can be solved (e.g., numerically), from which the behavior of the thermodynamically large system is to be extrapolated.

An important difference between the two Hamiltonians (18) and (19) is that the former always acts on a single-particle Hilbert space (as we only wrote the momentum operator for one particle – for N particles we should have written the sum $\sum_{i=1}^N \hat{p}_i^2$ over their N momentum operators instead), while the latter can act on any \mathcal{H}_N or the Fock space \mathcal{F} .

Let us understand the ground state of \hat{H}_μ at zero temperature, when acting on \mathcal{F} . When $\mu < 0$, it is just the vacuum $|0\rangle$, as occupying any state would cost energy. For $\mu > 0$ we have to separately consider the case of bosons from that of fermions: When considering bosons, an infinite number of particles would occupy the single-particle eigenstate of lowest energy ϵ_0 . In the case of fermions, every state can only be occupied once due to the Pauli exclusion principle. At the same time, it is only energetically advantageous to occupy single-particle eigenstate with negative energy $\epsilon_k < 0$. (We don't consider here the accidental case when one of the ϵ_k equals 0, in which case the ground state would be degenerate.) The fermionic zero-temperature ground state, the so-called Fermi sea (FS), is thus

$$|\text{FS}\rangle = \left(\prod_{k: \epsilon_k < 0} \hat{c}_k^\dagger \right) |0\rangle. \quad (21)$$

Finite-temperature properties of the system at inverse temperature $\beta = 1/(k_B T)$ can be computed from the partition function

$$Z_{\beta, \mu} = \text{Tr}_{\mathcal{F}} e^{-\beta \hat{H}_\mu}. \quad (22)$$

Equation (22) can be rationalized by recalling that the partition function is a sum of the unnormalized probabilities $e^{-\beta E_s}$ over all microstates s of the system, with associated energy E_s . Evaluating the trace $\text{Tr}_{\mathcal{F}}$ in the basis spanned by the eigenstates of \hat{H}_μ readily yields this connection. With Eq. (22) we compute the *grand canonical partition function*, i.e., the partition function for the grand canonical ensemble that is defined by not having a fixed particle number. This is reflected by the fact that we take the trace over the Fock space \mathcal{F} instead of a Hilbert space \mathcal{H}_N of fixed particle number N , and by the fact that the Hamiltonian contains the term $-\mu \hat{N}$. We indicate it with the subscript μ to remind us of the dependence on the chemical potential. The *canonical partition function* $Z_{\beta, N}$ for a system with fixed particle number N can be computed by dropping the latter term in the Hamiltonian and by restricting the trace in Eq. (22) over \mathcal{H}_N . Equation. (22) is a completely general formula that can be applied to any, possibly interacting, quantum

system. The finite-temperature expectation value of an operator \hat{O} is given by

$$\langle \hat{O} \rangle_{\beta, \mu} = \frac{1}{Z_{\beta, \mu}} \text{Tr}_{\mathcal{F}} \left[\hat{O} e^{-\beta \hat{H}_{\mu}} \right]. \quad (23)$$

As an example, we consider the momentum occupation number $\hat{n}_k := \hat{c}_k^\dagger \hat{c}_k$ for noninteracting particles in one dimension (an example would be the system governed by Hamiltonian (19)). We first compute the grand canonical partition function. To do so, we break up the trace

$$\text{Tr}_{\mathcal{F}} = \text{Tr}_{\mathcal{H}_0} + \text{Tr}_{\mathcal{H}_1} + \text{Tr}_{\mathcal{H}_2} + \cdots + \text{Tr}_{\mathcal{H}_N} + \cdots \quad (24)$$

to compute

$$\begin{aligned} Z_{\beta, \mu} &= \text{Tr}_{\mathcal{F}} e^{-\beta \hat{H}_{\mu}} \\ &= 1 + \sum_k e^{-\beta \varepsilon_k} + \sum_{k_1, k_2} e^{-\beta \varepsilon_{k_1}} e^{-\beta \varepsilon_{k_2}} + \cdots + \sum_{k_1, \dots, k_N} e^{-\beta \varepsilon_{k_1}} \times \cdots \times e^{-\beta \varepsilon_{k_N}} + \cdots \\ &= \prod_k \left(\sum_{n_k} e^{-\beta \varepsilon_k n_k} \right) \end{aligned} \quad (25)$$

For fermions, the momenta in each sum in the second line of Eq. (25) have to be all distinct $k_1 \neq k_2 \neq \cdots$ and the n_k -sum in the last line is only taken over $n_k = 0, 1$. For bosons, the sums are unrestricted and n_k runs over all nonnegative integers. As a result, we obtain

$$Z_{\beta, \mu}^{\text{F}} = \prod_k (1 + e^{-\beta \varepsilon_k}), \quad Z_{\beta, \mu}^{\text{B}} = \prod_k \frac{1}{1 - e^{-\beta \varepsilon_k}}, \quad (26)$$

for fermions and bosons, respectively. Note that $(1 + e^{-\beta \varepsilon_k})$ and $1/(1 - e^{-\beta \varepsilon_k})$ are the partition functions for a system of only a single degree of freedom (i.e., a system where the single-particle Hilbert space is restricted to only one momentum state). In general, the partition function of a system of independent degrees of freedom (i.e., degrees of freedom not coupled by the Hamiltonian through interactions), are given by the product over the partition functions of each of these degrees of freedom. Note that the form of the partition functions in Eq. (26) is general for any noninteracting fermion/boson system. The momentum k could be replaced by any label of the energy eigenvalues of the Hamiltonian acting on the single-particle Hilbert space.

Using the last line of Eq. (25), we can compute $\langle \hat{n}_k \rangle_{\beta, \mu}$ as

$$\langle \hat{n}_k \rangle_{\beta, \mu} = \frac{1}{Z_{\beta, \mu}} \left(\sum_{n_k} n_k e^{-\beta \varepsilon_k n_k} \right) \prod_{k' \neq k} \left(\sum_{n_{k'}} e^{-\beta \varepsilon_{k'} n_{k'}} \right) = -\frac{1}{\beta} \frac{\partial}{\partial \varepsilon_k} \ln Z_{\beta, \mu} \quad (27)$$

and obtain using Eq. (26)

$$\langle \hat{n}_k \rangle_{\beta, \mu}^F = \frac{1}{e^{\beta \varepsilon_k} + 1}, \quad \langle \hat{n}_k \rangle_{\beta, \mu}^B = \frac{1}{e^{\beta \varepsilon_k} - 1}, \quad (28)$$

for fermions and bosons, respectively. The functions $f_{F-D}(\varepsilon) := 1/(e^{\beta \varepsilon} + 1)$ and $f_{B-E}(\varepsilon) := 1/(e^{\beta \varepsilon} - 1)$ are the Fermi-Dirac and Bose-Einstein distribution functions, respectively. They dictate how the zero-temperature ground state occupations (i.e., the Fermi sea in the case of fermions) are smeared out by thermal fluctuations at finite temperature.

3. Thermodynamic potentials

From the partition function, one can derive the thermodynamic potentials that are useful quantities to characterize the state of a system and to compute its thermodynamic properties, such as the specific heat or the response to perturbations in the form of susceptibilities. Here, we will only discuss the quantities that will be relevant in the later course of the lecture. From the canonical partition function, we can compute the Helmholtz free energy as

$$F_{\beta, N} := -\frac{1}{\beta} \ln Z_{\beta, N}. \quad (29)$$

Analogously, from the grand canonical partition function, we can compute the grand potential as

$$\Omega_{\beta, \mu} := -\frac{1}{\beta} \ln Z_{\beta, \mu}. \quad (30)$$

The internal energy U is given by

$$U_N = -\frac{\partial}{\partial \beta} \ln Z_{\beta, N}, \quad U_\mu = -\frac{\partial}{\partial \beta} \ln Z_{\beta, \mu}, \quad (31)$$

and can be used to compute the specific heat

$$C = \frac{\partial U}{\partial T}. \quad (32)$$

We can further compute susceptibilities in of the system to external perturbations. If we perturb the system with an external parameter A and want to know how another parameter B of the system reacts to it, we compute

$$\chi_{AB} = -\frac{d^2 F}{dA dB}. \quad (33)$$

For example, the magnetic susceptibility of an isotropic system is obtained by setting $A = B = H$, where H is the magnetic field.

4. Spontaneous symmetry breaking

One of the central questions of condensed matter physics is to classify different phases of matter, study their properties and the transitions between them. The term “phase” can be used on different levels of rigor, but generically denotes a region in the space of external system parameters (such as applied electromagnetic fields, pressure, temperature etc) in which the properties of the system do not change. Hence, a phase is associated with some rigidity or stability against perturbations. At transitions between phases, system properties may change in a non-smooth fashion.

Some refined considerations apply to the definition of phases at zero temperature. Such phases and the transitions between them are purely associated with quantum fluctuations, rather than thermal fluctuations. Phase transitions at zero temperature are therefore called *quantum phase transitions*, or if happening at a point in the phase space this is called *quantum critical point*. At zero temperature, one can further distinguish gapless and gapped phases of matter, depending on whether or not the ground state is separated from all excited states by a finite energy gap in the thermodynamic limit.

One paradigm to classify phases of matter is that of *spontaneous symmetry breaking*, associated with the names Ginzburg and Landau. The system undergoes a phase transition from a high-symmetry, high-temperature phase, to a low-symmetry, low-temperature phase at a critical temperature phase T_c . Associated with the transition is a local observable, the so-called order parameter. Its expectation value is zero for $T > T_c$ and nonzero for $T < T_c$. One can deduce properties of the phase transition by general group-theoretic considerations. Denote by \mathcal{G} the symmetry group of the system above T_c and by $\mathcal{G}' \subset \mathcal{G}$ the symmetry group below T_c . The cardinality of the quotient \mathcal{G}/\mathcal{G}' determines the degeneracy of the ordered phase. The order parameter manifold is a representation of this quotient group. It can be either a continuous or discrete group.

Let us consider two examples, an Ising and a Heisenberg magnet. The Hamiltonian of the Ising model is given by

$$\hat{H}_I = -\frac{J}{2} \sum_{\langle i,j \rangle} \hat{s}_i \hat{s}_j \quad (34)$$

and the Hamiltonian of the Heisenberg model is given by

$$\hat{H}_H = -\frac{J}{2} \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \quad (35)$$

where the sum over i, j runs over the sites of a d dimensional square lattice and the $\langle i, j \rangle$ notation means that we only sum over nearest neighbor sites of the lattice. The coupling constant J is chosen to be positive for a ferromagnet and negative for an antiferromagnet.

We assume the Ising spins \hat{s}_i to be operators with a spectrum ± 1 that all commute with one another. The Heisenberg spins $\hat{\mathbf{S}}_i$ are an operator-valued 3-vector with components that obey

$$[\hat{S}_{i,\alpha}, \hat{S}_{j,\beta}] = i\epsilon_{\alpha,\beta,\gamma}\delta_{ij}\hat{S}_{i,\gamma}, \quad \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_i = S(S+1), \quad (36)$$

where S is a positive half-integer or integer constant. This renders the Ising problem completely classical (all operators entering the Hamiltonian commute), while the Heisenberg model could in principle show quantum-mechanical behavior.

In either case, we can guess the zero-temperature ground states for the ferromagnetic couplings $J > 0$. In the Ising case, they are given by

$$|+\rangle := |s_i = +1 \text{ on all sites}\rangle, \quad |-\rangle := |s_i = -1 \text{ on all sites}\rangle. \quad (37)$$

In the Heisenberg case, they are given by

$$|\mathbf{n}\rangle := |\mathbf{n} \cdot \hat{\mathbf{S}} = +1 \text{ on all sites}\rangle, \quad (38)$$

where \mathbf{n} is a unit vector in any chosen direction. These are two states for the Ising case and a continuum of states that represent the rotation group $SO(3)$ in spin space. It is not a coincidence that we obtain these degenerate ground states. Hamiltonian (34) has a so-called global \mathbb{Z}_2 symmetry: It is invariant under the spin-flip $\hat{s}_i \rightarrow -\hat{s}_i \forall i$. The Hamiltonian (35) has a global $SO(3)$ symmetry, because the spin-rotation $\prod_i e^{i\mathbf{w} \cdot \hat{\mathbf{S}}_i / S}$, that rotates all spins around the axis \mathbf{w} by an amount $|\mathbf{w}|$ commutes with the Hamiltonian for all choices of the constant vector \mathbf{w} . For that reason all states at a given energy must span a subspace of the Hilbert space that is invariant under the application of the symmetry operation. Therefore, if $|+\rangle$ is a ground state, there must be a degenerate ground state $|-\rangle$, and likewise for the Heisenberg case. In fact the Hamiltonians (34) and (35) have larger symmetry groups that we denote by \mathcal{G}_I and \mathcal{G}_H , respectively, and which includes lattice translations and spatial rotations, for example. We factorize these groups as $\mathcal{G}_I = \mathcal{G}'_I \times \mathbb{Z}_2$ and $\mathcal{G}_H = \mathcal{G}'_H \times SO(3)$ into a part $\mathcal{G}'_{H,I}$ of which each ground state is a trivial representation and the nontrivial part discussed above.

In a real system, the symmetries are never exactly present, but broken by small local perturbations. (The emphasis on locality comes from the physical requirement that terms in the Hamiltonian should not couple degrees of freedom that are far away, or if they do so, then with a strength that decays sufficiently fast with their distance.) For example, the spin-rotation symmetry can be broken by magnetic impurities, or even by coupling to the earth's magnetic field. As a result of these perturbations, the system will choose one of the (almost) degenerate ground states. Once chosen, this ground state is robust, even if the perturbation is removed or reversed, because changing between, say, $|+\rangle$ and $|-\rangle$ requires reorganizing a macroscopic number of degrees of freedom. This constitutes a large energy barrier as domain walls have to propagate through the system. In fact, this process has vanishing probability if the system size is taken to infinity (the thermodynamic limit).

The process of spontaneous symmetry breaking can be cast in more rigorous terms as follows. We define an order parameter, the magnetization

$$\widehat{M} = \frac{1}{N} \sum_i \widehat{s}_i, \quad \widehat{\mathbf{M}} = \frac{1}{N} \sum_i \widehat{\mathbf{S}}_i, \quad (39)$$

where N is the number of lattice sites. We further add perturbations to the Hamiltonians

$$\widehat{H}_{I,h} = \widehat{H}_I + \sum_i h \widehat{s}_i, \quad \widehat{H}_{H,\mathbf{H}} = \widehat{H}_I + \sum_i \mathbf{H} \cdot \widehat{\mathbf{S}}_i \quad (40)$$

that break the symmetry subgroup $\mathcal{G}_{I,H}/\mathcal{G}'_{I,H}$. Spontaneous symmetry breaking occurs if

$$0 \neq \lim_{h \rightarrow 0} \lim_{N \rightarrow \infty} \langle \widehat{M} \rangle_{\beta, H_{I,h}}, \quad 0 \neq \lim_{\mathbf{H} \rightarrow 0} \lim_{N \rightarrow \infty} \langle \widehat{\mathbf{M}} \rangle_{\beta, H_{H,\mathbf{H}}}, \quad (41)$$

while it is zero if the limits were taken in the reverse order. The expectation value at finite inverse temperature β was defined in Eq. (23). Equation (41) holds for the ferromagnetic case $J > 0$. For the antiferromagnet, we would need to use the staggered magnetization as an order parameter and apply a staggered perturbation. To be able to define a staggered magnetization, it is important that our square lattice is bipartite in any dimension, i.e., the sites can be divided into two sets A and B such that all nearest neighbors of a site in A are in B . For instance, a triangular lattice in $d = 2$ is not bipartite and we say the antiferromagnet is geometrically frustrated on this lattice. We will study these magnetic orders in more detail in Chapter V.

An important distinction is made between spontaneous symmetry breaking of a discrete and a continuous symmetry group. The latter are accompanied by Goldstone modes (one

mode per generator of a continuous symmetry), which are gapless excitations above the symmetry-breaking ground state manifold. This implies that the ground state of the Ising ferromagnet can have (and has in fact) a finite gap to all other excitations, while the ground state of the Heisenberg ferromagnet has gapless excitations that are spin-wave deformations of the ferromagnetic pattern.

A natural question is: Under which conditions can spontaneous symmetry breaking occur? This question is answered by the Mermin-Wagner theorem, stating that a continuous symmetry cannot be spontaneously broken at any finite temperature in $d \leq 2$ (with sufficiently short-ranged interactions). In $d = 2$, a continuous symmetry can be spontaneously broken at zero temperature. In $d = 1$, a continuous symmetry can never be broken spontaneously.

5. Mean-field approximation

States with spontaneously broken symmetry are often treated within the so-called mean-field approximation. Above, we have seen that in a symmetry-broken ground state, observables that have a vanishing expectation value in any *eigenspace* of the Hamiltonian (which is necessarily invariant under the symmetries of the system) acquire a non-vanishing expectation value. For the example of the spin operator in the Ising model, we can relate it to the classical magnetization M of the system

$$\hat{s}_i = M + \delta\hat{s}_i. \quad (42)$$

The mean-field approximation consists of dropping higher orders of the operators $\delta\hat{s}_i$ from the Hamiltonian, so that the system becomes soluble.

We will go through this mean-field calculation for the example of the Ising model, where $\delta\hat{s}_i = \hat{s}_i - M$ for all lattice sites i . The Hamiltonian is rewritten as

$$\begin{aligned} \hat{H} &= -\frac{J}{2} \sum_{\langle i,j \rangle} [M + (\hat{s}_i - M)][M + (\hat{s}_j - M)] - h \sum_i \hat{s}_i \\ &= -J \sum_i \left(zM\hat{s}_i - z\frac{M^2}{2} \right) - h \sum_i \hat{s}_i + \mathcal{O}(\delta\hat{s}_i\delta\hat{s}_j), \end{aligned} \quad (43)$$

where z is the coordination number of the nearest neighbors on the lattice (on a hypercubic lattice $z = 2d$). Neglecting the last term is justified if $\langle \delta\hat{s}_i\delta\hat{s}_j \rangle / (\langle \delta\hat{s}_i \rangle \langle \delta\hat{s}_j \rangle) = \langle \delta\hat{s}_i\delta\hat{s}_j \rangle / M^2 \ll$

1. The mean field Hamiltonian

$$\hat{H}_{\text{mf}} = - \sum_i \hat{s}_i h_{\text{eff}} - NJ \frac{z}{2} M^2 + \mathcal{O}(\delta \hat{s}_i \delta \hat{s}_j), \quad (44)$$

which is the Hamiltonian for an ideal paramagnet (a collection of independent spins) in a magnetic field $h_{\text{eff}} = JzM + h$. The partition function for this Hamiltonian is

$$\begin{aligned} Z_N(\beta, M, h) &= e^{-\beta JzM^2 N/2} \prod_i \sum_{s_i = \pm 1} e^{\beta h_{\text{eff}} s_i} \\ &= e^{-\beta JzM^2 N/2} [2 \cosh(\beta h_{\text{eff}})]^N, \end{aligned} \quad (45)$$

from which we find the free energy

$$F(\beta, M, h) = -\beta^{-1} \log Z_N = NJ \frac{z}{2} M^2 - N\beta^{-1} \log [2 \cosh(\beta h_{\text{eff}})]. \quad (46)$$

To find out whether a stable mean-field solution for M exists, we are looking for a minimum of the free energy at finite M . Indeed

$$0 = \frac{\partial F}{\partial M} = NJzM - NJz \tanh(\beta h_{\text{eff}}) \quad (47)$$

has such a solution iff the self-consistency equation

$$M = \tanh[\beta(JzM + h)] \quad (48)$$

has one. We particularize on the case of zero magnetic field, and expand the \tanh to linear order in M in order to find the phase boundary. Solutions to Eq. (48) exist when the slope of the function on the righthand side at $M = 0$ is larger than 1. This linearized self-consistency equation

$$M = \beta JzM \quad (49)$$

yields from this condition the critical temperature

$$T_c = Jz/k_B. \quad (50)$$

B. Linear response

Linear response studies the change in an observable \hat{A} due to a small change $\hat{H}_{\hat{B}}(t)$ in the static Hamiltonian \hat{H}_0 of the system. The perturbation can be time-dependent with, say, a single frequency ω and is adiabatically slowly switched on, i.e., the time-dependence

is taken to be $\hat{H}_{\hat{B}}(t) = \hat{B}e^{-i\omega t + \eta t}$ with η a small positive real number. The Schroedinger equation for the perturbation is then

$$\begin{aligned} i\frac{d}{dt}\hat{A} &= [\hat{A}, \hat{H}_0 + \hat{H}_{\hat{B}}(t)] \\ &= [\hat{A}, \hat{H}_0] + [\hat{A}, \hat{B}]e^{-i\omega t + \eta t}. \end{aligned} \quad (51)$$

Taking the thermal average of this equation $\langle \hat{A} \rangle = \text{Tr}[\hat{A}e^{-\beta\hat{H}_0}]/\text{Tr}[e^{-\beta\hat{H}_0}]$ yields

$$(\omega + i\eta)\langle \hat{A} \rangle = \langle [\hat{A}, \hat{H}_0] \rangle + \langle [\hat{A}, \hat{B}] \rangle, \quad (52)$$

which is subsequently solved to linear order in \hat{B} . Here it was assumed that the expectation values of \hat{A} and its commutators acquire the same time dependence $e^{-i\omega t + \eta t}$ as the perturbation, and we are only probing this one Fourier component.

Consider the example of perturbing a free electrons gas (a metal in condensed matter language) with a spatially and temporally varying potential (e.g., caused by an external electric field). We are interested in the response of the electron density. The density operator in momentum space is given by

$$\begin{aligned} \hat{\rho}_{\mathbf{q}} &= \int d\mathbf{r} \hat{\phi}^\dagger(\mathbf{r}) \hat{\phi}(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} \\ &= \frac{1}{\Omega} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}+\mathbf{q}} \\ &\equiv \frac{1}{\Omega} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k},\mathbf{q}}. \end{aligned} \quad (53)$$

Then setting corresponds to

$$\hat{H}_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}}, \quad \hat{H}_{\hat{B}} = \hat{\rho}_{\mathbf{q}}^\dagger V(\mathbf{q}, \omega) e^{-i\omega t + \eta t} = \frac{1}{\Omega} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k},\mathbf{q}}^\dagger V(\mathbf{q}, \omega) e^{-i\omega t + \eta t} \quad (54)$$

and $\hat{A} = \hat{\rho}_{\mathbf{q}}$. Using $[AB, BD] = A\{B, C\}D - \{A, C\}BD - C\{A, D\}B + CA\{B, D\}$ we obtain the commutator

$$[\hat{\rho}_{\mathbf{k},\mathbf{q}}, \hat{\rho}_{\mathbf{k}',\mathbf{q}}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'} (\hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} - \hat{c}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{c}_{\mathbf{k}+\mathbf{q}}) \quad (55)$$

and

$$[\hat{\rho}_{\mathbf{k},\mathbf{q}}, \hat{\rho}_{\mathbf{k}',\mathbf{0}}^\dagger] = (\delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'} - \delta_{\mathbf{k},\mathbf{k}'}) \hat{\rho}_{\mathbf{k},\mathbf{q}} \quad (56)$$

we have

$$(\omega + i\eta)\langle \hat{\rho}_{\mathbf{k},\mathbf{q}} \rangle = (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\langle \hat{\rho}_{\mathbf{k},\mathbf{q}} \rangle + (\langle \hat{n}_{\mathbf{k}+\mathbf{q}} \rangle^F - \langle \hat{n}_{\mathbf{k}} \rangle^F) V(\mathbf{q}, \omega), \quad (57)$$

where $\langle \hat{n}_{\mathbf{k}} \rangle^F = \langle \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} \rangle$ is determined by the Fermi-Dirac distribution. Thus, summing over \mathbf{k} , we find the change in the electron density due to the external perturbation as

$$\delta\rho(\mathbf{q}, \omega) = \frac{1}{\Omega} \sum_{\mathbf{k}} \langle \hat{\rho}_{\mathbf{k}, \mathbf{q}} \rangle = \chi_0(\mathbf{q}, \omega) V(\mathbf{q}, \omega), \quad (58)$$

where we defined the linear response function as

$$\chi_0(\mathbf{q}, \omega) = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{\langle \hat{n}_{\mathbf{k}+\mathbf{q}} \rangle^F - \langle \hat{n}_{\mathbf{k}} \rangle^F}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega - i\eta}, \quad (59)$$

which is known as the *Lindhard* form.

C. Symmetries in condensed matter

1. Non-local vs. local, unitary vs. antiunitary

In particle physics, the fundamental symmetries are Lorentz symmetry, \mathcal{C} (charge conjugation), \mathcal{P} (parity or inversion), \mathcal{T} (time-reversal symmetry), as well as the gauge symmetries of the standard model. Of these symmetries, only \mathcal{T} and \mathcal{P} are important in condensed matter physics. Wigner proved that any symmetry is either represented by antiunitary or unitary operators in quantum mechanics (i.e., by operators that contain complex conjugation or not). Time-reversal symmetry is of the antiunitary kind. To see this, consider the Schrödinger equation: In order to flip ∂_t to $-\partial_t$ in general, the only option we have is to send $i \rightarrow -i$. The fundamental representation of time reversal on systems with bosonic degrees of freedom or ‘spinless’ fermions is $\mathcal{T} = K$. For spin-1/2 fermions, in contrast $\mathcal{T} = K(i\sigma_y)$, where σ_y is the second Pauli matrix acting on each fermion’s spin degree of freedom. Most other symmetries that we will be concerned with are unitary (another fundamental exception is the charge conjugation symmetry \mathcal{C} in high energy physics mentioned above).

A *local* unitary symmetry U can be written as $U = U_1 U_2 \cdots U_n$, where each U_i acts only on a small region in space and the number of operators n grows proportional to the system size if the latter is taken to infinity. As an example, consider the spin rotations $R_{\boldsymbol{\alpha}} = \prod_{\text{spins } i} \exp[i\boldsymbol{\alpha} \cdot \mathbf{S}_i]$, that would rotate all spins in the Heisenberg model that we discussed above by the same amount.

In contrast, a *nonlocal* unitary symmetry cannot be decomposed in the above way. Typical examples for such symmetries include spatial symmetries like reflections, rotations of configuration space.

Such spatial symmetries shift the degrees of freedom (like lattice sites) around in space, but also act on atomic orbitals and on the spin degree of freedom of an electron on each site. For the latter part of their action, inversion (I), mirror $M_{\hat{e}}$, and rotations R_{α} act on a spin-1/2 as

$$I = \sigma_0, \quad M_{\hat{e}} = i\hat{e} \cdot \boldsymbol{\sigma}, \quad R_{\alpha} = \exp[i\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}/2]. \quad (60)$$

As a side remark, time-reversal (and other anti-unitary symmetries) can be seen as a non-local symmetry, since the complex conjugation acts non-locally. However, up to this subtlety it is acting as a local symmetry. Time-reversal has to commute with all spatial symmetries like rotations, mirror reflections, and inversion.

Finally, in condensed matter Lorentz symmetry is broken by the existence of a crystal lattice, that is fixed (or vibrates only in small perturbations – phonons and sound waves) and therefore the most prominent example of a broken symmetry state. However, the Lorentz group is broken down to a discrete subgroup rather than completely broken in a crystal. This makes our life a lot easier and we will explore these remaining symmetry properties of a crystal in the next section.

2. Symmetries of a crystal

A *crystal* is regular lattice of repeating structures (the unit cell) attached to all positions \mathbf{R}_n

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \quad (61)$$

with linearly independent basis vectors \mathbf{a}_i , $i = 1, 2, 3$ and $\mathbf{n} \in \mathbb{Z}^3$.

The *space group of a crystal* \mathcal{R} is the group of all symmetry operations that leave the crystal invariant: translations, rotations, inversion, reflections, and combinations thereof. [Recall that a group \mathcal{G} is a set of elements $a, b, c, \dots \in \mathcal{G}$ with a multiplication \star such that it is: closed $a \star b = c \in \mathcal{G}$; associative $a \star (b \star c) = (a \star b) \star c$; \exists identity e , such that $\forall a$, $a \star e = e \star a = a$; $\forall a \exists$ an inverse a^{-1} such that $a \star a^{-1} = a^{-1} \star a = e$. If $a \star b = b \star a$ the group is Abelian, otherwise it is non-Abelian; space groups are often non-Abelian, as for example rotations do not commute.] In 2D there are 17 space groups (the so-called wallpaper groups), in 3D there are 230 space groups. These counts apply to systems with time-reversal symmetry, in magnetic systems the numbers are larger.

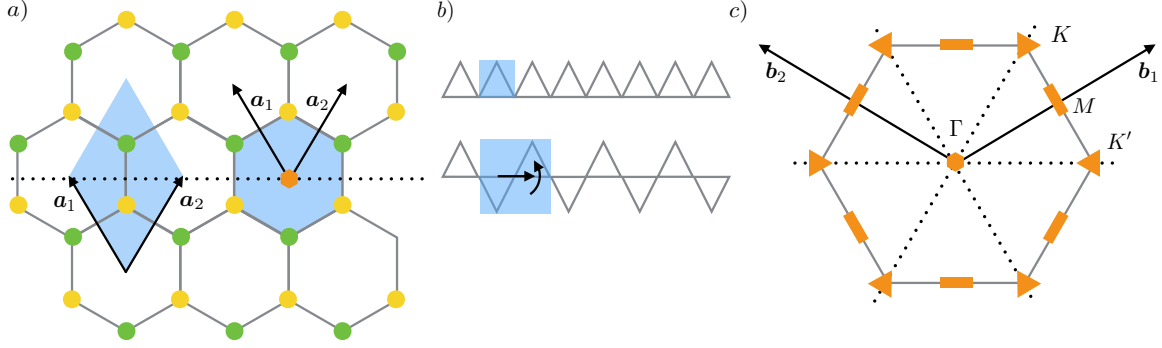


Figure 1. a) The honeycomb lattice with two different choices of unit cells. The lattice is not primitive, i.e., the repeating unit cell contains more than one (here, two) sites marked in green and yellow. They are called the two sublattices of the honeycomb lattice. The hexagonal unit cell is the Wigner-Seitz cell. b) Symmorphic and nonsymmorphic one-dimensional lattice with unit cells marked in blue. The nonsymmorphic symmetry of the latter is a glide mirror for which half of a lattice translation is combined with a reflection about the one-dimensional axis of the chain. c) Brillouin zone of the honeycomb lattice. High-symmetry points are marked. The Γ point is also left invariant by the six-fold rotational symmetry, the M point has two-fold rotational symmetry and the K point has three-fold rotational symmetry. Planes left invariant under the mirror reflection about the dotted line in a) are marked by dotted lines.

The unit cell of a lattice is not fixed uniquely. The Wigner-Seitz cell is a specific choice that consists of the region of space that is closer to a given lattice point than to any other. [See Fig. 1 a)]

Using the so-called Wigner notation, we can write a general spatial symmetry transformation of a crystal as a combination of a translation and another spatial symmetry

$$\mathbf{r}' = g\mathbf{r} + \mathbf{a} \equiv \{g|\mathbf{a}\}\mathbf{r}, \quad (62)$$

where the elements g form the (smaller) point group \mathcal{P} . It is tempting to think that all allowed operations in a crystal are either *translations* $\{E|\mathbf{a}\}$ or *rotations, mirror reflections, inversions* $\{g|\mathbf{0}\}$ in which case $\mathbf{R} = \mathcal{P} \times \text{trn}$, i.e., the space group is the direct product of the point group elements and translations. This holds for so-called *symmorphic* space groups (in 3D these are 73 of the 230). The remaining *nonsymmorphic* space groups also contain *screw rotations* and *glide mirror* symmetries $\{g|\mathbf{a}\}$, where \mathbf{a} is a fractional lattice

Table I. List of all space groups in 3D time-reversal symmetric crystals.

crystal system	angles	equal sides	space group numbers	point groups
triclinic	α, β, γ	0	1–2	$C_1, C_{\bar{1}}$
monoclinic	$\frac{\pi}{2}, \frac{\pi}{2}, \beta$	0	3–15	C_2, C_s, C_{2h}
orthorhombic	$\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}$	0	16–74	D_2, C_{2v}, D_{2h}
tetragonal	$\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}$	2	75–142	$C_4, S_4, C_{4h}, D_4, C_{4v}, D_{2d}, D_{4h}$
trigonal	$\frac{\pi}{2}, \frac{\pi}{2}, 4\frac{\pi}{3}$	2	143–167	$C_3, S_6, D_3, C_{3v}, D_{3d}$
hexagonal	$\frac{\pi}{2}, \frac{\pi}{2}, 4\frac{\pi}{3}$	2	168–194	$C_6, C_{3h}, C_{6h}, D_6, C_{6v}, D_{3h}, D_{6h}$
cubic	$\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}$	3	195–230	T, T_h, O, T_d, O_h

translation. [See Fig. 1 b)] A screw rotation is a rotation combined with a translation along the rotation axis. A glide mirror is a mirror reflection combined with a translation within the mirror plane. The associative multiplication rule for symmetry transformations in the Wigner notation is

$$\{g|\mathbf{a}\}\{g'|\mathbf{a}'\} = \{gg'|\mathbf{a}' + \mathbf{a}\}. \quad (63)$$

The group of lattice translations $\{E|\mathbf{R}_n\}$ is an Abelian subgroup of \mathcal{R} .

3. Reciprocal space

Discrete translational symmetry of a system implies that eigenstates of the Hamiltonian can be labelled by the eigenvalues of the translation operator, which are the momenta \mathbf{k} . We will now explore the reciprocal space, in which the \mathbf{k} live.

If we are interested to evaluate a function f only on lattice points \mathbf{R}_n , i.e., in discretized space, two terms $f_{\mathbf{k}}$ and $f_{\mathbf{k}'}$ in a Fourier expansion

$$f(\mathbf{R}_n) = \sum_{\mathbf{k}} f_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_n} \quad (64)$$

are linearly dependent if $e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_n} = 1$ for all \mathbf{R}_n in the lattice. This allows to define the reciprocal lattice as the collection of points \mathbf{G} in momentum space with

$$1 = e^{i\mathbf{G} \cdot \mathbf{R}_n}, \quad \forall \mathbf{R}_n. \quad (65)$$

The reciprocal lattice is spanned by \mathbf{b}_i , $i = 1, 2, 3$ with

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)} \quad (66)$$

for which $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$

$$\mathbf{G}_m = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3. \quad (67)$$

A function g that is expanded as

$$g(\mathbf{r}) = \sum_{\mathbf{G}} g_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}} \quad (68)$$

and evaluated at \mathbf{r} in continuous real space will have the periodicity of the lattice. If we have a chance to probe such a lattice-periodic function $g(\mathbf{r})$ with a plane wave, say in a scattering experiment, we are frequently compute

$$\begin{aligned} F[g] &= \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} g(\mathbf{r}) \\ &= \sum_{\mathbf{R}} \int_{\text{unit cell}} d\mathbf{x} e^{i\mathbf{k} \cdot (\mathbf{x} + \mathbf{R})} g(\mathbf{x} + \mathbf{R}) \\ &= \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} S(\mathbf{k}), \end{aligned} \quad (69)$$

where

$$S(\mathbf{k}) = \int_{\text{unit cell}} d\mathbf{x} e^{i\mathbf{k} \cdot \mathbf{x}} g(\mathbf{x}) \quad (70)$$

is called the *structure factor*.

The Brillouin zone (BZ) is the unit cell of the reciprocal lattice. Certain points, lines, or planes in the BZ are left invariant under some of the point group symmetry operations. By definition (since \mathbf{k} are the eigenvalues of a translation operator), translations leave each point in reciprocal space invariant. Mirror reflections leave the planes perpendicular to the mirror normal invariant. Inversion leaves the so-called TRIM points (time-reversal invariant momenta) $\mathbf{k} = \mathbf{0}$ (the Γ point), $\mathbf{k} = \mathbf{b}_1/2$, $\mathbf{k} = \mathbf{b}_2/2$, $\mathbf{k} = \mathbf{b}_3/2$, $\mathbf{k} = \mathbf{b}_1/2 + \mathbf{b}_2/2$, $\mathbf{k} = (\mathbf{b}_1 + \mathbf{b}_3)/2$, $\mathbf{k} = (\mathbf{b}_2 + \mathbf{b}_3)/2$, $\mathbf{k} = (\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3)/2$ invariant, because it maps \mathbf{k} to $-\mathbf{k}$, but $\mathbf{k} \equiv \mathbf{k} + \mathbf{G}$. The same points are left invariant by the time-reversal transformation. Rotations leave the points along some lines parallel to the rotation axis invariant. [See Fig. 1 c) for the honeycomb lattice as a 2D example.]

The group of symmetry operations that leave a point, line or plane in momentum space invariant is called its *little group*.

III. NONINTERACTING ELECTRON SYSTEMS

A. Bloch's theorem

We explore the consequences of the Abelian subgroup of translations of the point group of a crystal. A Hamiltonian \hat{H} that commutes with all translation operators $\hat{T}_{\mathbf{R}_n}$, i.e., $[\hat{H}, \hat{T}_{\mathbf{R}_n}] = 0$ is considered. The translation operator is defined through its action on single-particle operators in the position basis

$$\hat{T}_{\mathbf{R}_n} \hat{\phi}^\dagger(\mathbf{r}) \hat{T}_{\mathbf{R}_n}^{-1} = \hat{\phi}^\dagger(\mathbf{r} + \mathbf{R}_n), \quad \hat{T}_{\mathbf{R}_n} \hat{\phi}(\mathbf{r}) \hat{T}_{\mathbf{R}_n}^{-1} = \hat{\phi}(\mathbf{r} + \mathbf{R}_n), \quad \hat{T}_{\mathbf{R}_n}^{-1} = \hat{T}_{-\mathbf{R}_n}. \quad (71)$$

We are, however, going to formulate things in first quantized language now. Consider the single particle Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}), \quad (72)$$

with the periodic potential $V(\mathbf{r} + \mathbf{R}_n) = V(\mathbf{r})$ that could stem from a lattice of ions. \hat{H} and $\hat{T}_{\mathbf{R}_n}$ are all commuting and hence have a common eigenbasis. Bloch's theorem says that the eigenstates of $\hat{T}_{\mathbf{R}_n}$ have eigenvalues on the unit circle in the complex plane in order not to blow up and to be extended. More precisely, the eigenstates of $\hat{T}_{\mathbf{a}_i}$ are plane waves

$$\hat{T}_{\mathbf{a}_i} |\mathbf{k}, m\rangle = e^{i\mathbf{k} \cdot \mathbf{a}_i} |\mathbf{k}, m\rangle, \quad (73)$$

where m labels a possible degeneracy of the eigenspace.

A wave-function (notice the subtle distinction between wave function and state) of the form

$$\langle \mathbf{r} | \mathbf{k}, m \rangle \equiv \psi_{m,\mathbf{k}} = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{m,\mathbf{k}}(\mathbf{r}) \equiv \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k} \cdot \mathbf{r}} \langle \mathbf{r} | u_{\mathbf{k},m} \rangle \quad (74)$$

satisfies this property if

$$u_{m,\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) = u_{m,\mathbf{k}}(\mathbf{r}) \quad (75)$$

because then

$$\psi_{m,\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) = e^{i\mathbf{k} \cdot \mathbf{R}_n} \psi_{m,\mathbf{k}}(\mathbf{r}). \quad (76)$$

We choose $|\mathbf{k}, m\rangle$ to also diagonalize \hat{H}

$$\hat{H} |\mathbf{k}, m\rangle = \epsilon_{n,\mathbf{k}} |\mathbf{k}, m\rangle, \quad (77)$$

where m is the so-called band index, \mathbf{k} is the pseudo-momentum, and $u_{m,\mathbf{k}}(\mathbf{r})$ the Bloch wavefunction. Because $e^{i\mathbf{k} \cdot \mathbf{R}_n} = e^{i(\mathbf{k} + \mathbf{G}_m) \cdot \mathbf{R}_n}$, two momenta that differ by a reciprocal lattice

vector \mathbf{G}_m are in the same eigenspace of the translation operator and we can restrict \mathbf{k} to the first BZ. Using

$$\hat{\mathbf{p}}|\mathbf{k}, m\rangle = \hat{\mathbf{p}}e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|u_{\mathbf{k},m}\rangle = e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}(\hat{\mathbf{p}} + \mathbf{k})|u_{\mathbf{k},m}\rangle, \quad (78)$$

we find the *Bloch equation*

$$\left[\frac{(\hat{\mathbf{p}} + \mathbf{k})^2}{2m} + V(\hat{\mathbf{r}}) \right] |u_{\mathbf{k},m}\rangle = \epsilon_{m,\mathbf{k}} |u_{\mathbf{k},m}\rangle, \quad (79)$$

which has now to be solved for periodic states, i.e., $T_{\mathbf{R}_n}|u_{\mathbf{k},m}\rangle = |u_{\mathbf{k},m}\rangle$ only. (Notice that, had we not set $\hbar = 1$, the momentum shift would read $\hbar\mathbf{k}$.) Taking the overlap with a position eigenstate from the left, we obtain the alternate form in terms of wave functions

$$\left[\frac{(-i\nabla_{\mathbf{r}} + \mathbf{k})^2}{2m} + V(\mathbf{r}) \right] u_{\mathbf{k},m}(\mathbf{r}) = \epsilon_{m,\mathbf{k}} u_{\mathbf{k},m}(\mathbf{r}). \quad (80)$$

The fact that differential equations involving periodic functions have solutions that have the same periodicity is a theorem named after Gaston Floquet (Floquet theory) in math. It was rediscovered in the condensed matter context by Felix Bloch. In physics, Floquet's name is attached to the study of systems that are driven periodically in time.

We will now use two strategies to attack this problem, the nearly free electron approximation and the tight-binding approximation.

B. Nearly free electron approximation

In the nearly free electron approximation we consider electrons in a weak potential that has the periodicity of the lattice

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}. \quad (81)$$

We want to solve the Bloch equation using perturbation theory in $V(\mathbf{r})$. In configuration space, the potential is a real function. If in addition $V(\mathbf{r}) = V(-\mathbf{r})$ (inversion symmetry), then $V_{\mathbf{G}} = V_{\mathbf{G}}^* = V_{-\mathbf{G}}$. Using the periodicity of the Bloch wave function, we can expand

$$u_{\mathbf{k},m}(\mathbf{r}) = \sum_{\mathbf{G}} c_{\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} \quad (82)$$

to obtain

$$\left[\frac{(\mathbf{k} - \mathbf{G})^2}{2m} - \epsilon_{m,\mathbf{k}} \right] c_{\mathbf{G}} + \sum_{\mathbf{G}'} V_{\mathbf{G}' - \mathbf{G}} c_{\mathbf{G}'} = 0, \quad (83)$$

which presents an eigenvalue problem for the matrix $V_{\mathbf{G}',\mathbf{G}} = V_{\mathbf{G}'-\mathbf{G}}$ in infinite dimensions. The zeroth order energy eigenvalues are given by the free electron parabolas

$$\epsilon_{\mathbf{G},\mathbf{k}}^{(0)} = \frac{(\mathbf{k} - \mathbf{G})^2}{2m}, \quad (84)$$

where we can use the reciprocal lattice vectors \mathbf{G} as band labels. The first order result is given by

$$\epsilon_{\mathbf{G},\mathbf{k}}^{(1)} = \epsilon_{\mathbf{G},\mathbf{k}}^{(0)} + \sum_{\mathbf{G}' \neq \mathbf{G}} \frac{|V_{\mathbf{G}-\mathbf{G}'}|^2}{\epsilon_{\mathbf{G},\mathbf{k}}^{(0)} - \epsilon_{\mathbf{G}',\mathbf{k}}^{(0)}}, \quad (85)$$

valid if the bands are nondegenerate. If bands are degenerate, as it happens for example at the zone boundary, we have to resort to degenerate perturbation theory (as we will exemplify below).

1D example: Consider a 1D system perturbed by the potential with general coefficients $V_G \ll G^2/(2m)$, where $G = nb$ and b the unit vector spanning the reciprocal lattice. Let us first compute the corrections to the lowest band for small k , i.e., near the zone center $k \ll b$. We obtain

$$\begin{aligned} \epsilon_{0,k}^{(1)} &= \frac{k^2}{2m} - \sum_{G \neq 0} \frac{|V_G|^2}{[(k - G)^2 - k^2]/(2m)} \\ &\approx \frac{k^2}{2m^*} + E_0, \end{aligned} \quad (86)$$

which we recast into a parabolic term with altered mass (the so-called effective mass) and an overall energy shift

$$\frac{1}{m^*} = \frac{1}{m} \left[1 - 4 \sum_{G \neq 0} \left(\frac{2m|V_G|}{G^2} \right)^2 \right], \quad E_0 = - \sum_{G \neq 0} \frac{2m|V_G|^2}{G^2}. \quad (87)$$

Next, let us consider what happens to the next-higher bands $G = \pm b$ at the zone center, i.e., for $k \ll b$. This problem has to be tackled with degenerate perturbation theory, for $\epsilon_{b,k}^{(0)}$ and $\epsilon_{-b,k}^{(0)}$ are degenerate at $k = 0$. Degenerate perturbation theory amounts to diagonalizing the Bloch equation in the degenerate subspace first (note that we cannot use the reciprocal lattice vectors anymore as a label for the eigenstates, the perturbation is now really mixing them)

$$\begin{pmatrix} \frac{(k-b)^2}{2m} - \epsilon_k & V_{-2b} \\ V_{2b} & \frac{(k+b)^2}{2m} - \epsilon_k \end{pmatrix} \begin{pmatrix} c_b \\ c_{-b} \end{pmatrix} = 0. \quad (88)$$

The characteristic equation of the above yields the eigenvalues

$$\begin{aligned}\epsilon_{\pm,k} &= \frac{1}{2} \left\{ \frac{(k+b)^2 + (k-b)^2}{2m} \pm \sqrt{\left[\frac{(k+b)^2 + (k-b)^2}{2m} \right]^2 + 4|V_{2b}|^2} \right\} \\ &= \frac{k^2}{2m_{\pm}^*} \pm |V_{2b}| + \frac{b^2}{2m},\end{aligned}\tag{89}$$

with the effective mass

$$\frac{1}{m^*} = \frac{1}{m} \left[1 \pm \frac{b^2}{m|V_{2b}|} \right],\tag{90}$$

which due to $|V_{2b}| \ll b^2/(2m)$ have opposite sign. Thus the two bands obtain opposite curvature. A *band gap* has opened. At $k = 0$, where the nontrivial part of the above matrix is proportional to σ_1 , the eigenstates are given by $c_b = \pm c_{-b}$ yielding the real-space Bloch wave functions

$$u_{k=0,+}(x) = \cos(bx), \quad u_{k=0,-}(x) = \sin(bx),\tag{91}$$

i.e., they are even and odd under the parity operation.

We can analyze the momenta at the zone boundary in a similar fashion using degenerate perturbation theory, where we would likewise find the opening of a band gap. [See Fig. 2 a).]

C. Tight-binding approximation

We are now attempting to solve the Bloch equation in exactly the opposite limit, where electrons are bound to a regular lattice of ionic potentials and the quantum mechanical tunneling process of an electron between two atoms is seen as the perturbation. This so-called tight-binding approximation is of much higher practical relevance than the nearly free electron approximation.

Let us consider atoms positioned on sites \mathbf{R}_i that could form a simple lattice or a lattice with a basis. An isolated atom at \mathbf{R} is described by a Hamiltonian

$$\hat{H}_{\text{atom},\mathbf{R}} = \frac{\hat{p}^2}{2m} + V_{\text{atom}}(\hat{\mathbf{r}} - \mathbf{R})\tag{92}$$

which we can formally diagonalize

$$\hat{H}_{\text{atom},\mathbf{R}}|\alpha, \mathbf{R}\rangle = \epsilon_{\alpha}|\alpha, \mathbf{R}\rangle,\tag{93}$$

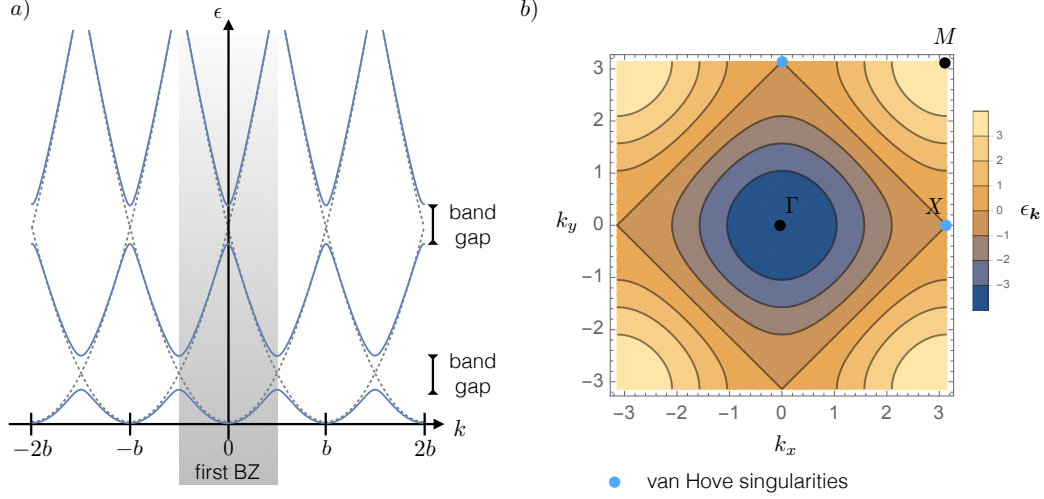


Figure 2. a) Band structure of a 1D system obtained within the nearly free electron approximation. b) Band structure of a tight-binding model on the square lattice with only nearest-neighbor hopping. The blue dots mark the position of van Hove singularities where the density of states diverges. Together with the black high-symmetry points, they form the set of independent time-reversal invariant momenta in this BZ. The contours correspond to the different Fermi lines as the band filling is changed.

noting that the eigenstates (the atomic orbitals) in the position basis $\langle \mathbf{r} | \alpha, \mathbf{R} \rangle$ are functions of $\mathbf{r} - \mathbf{R}$ only. We understand V_{atom} as the (rotationally symmetric) atomic potential and subsume all quantum numbers (orbital/angular momentum and spin) in the index α .

A single-particle Hamiltonian of the whole lattice is then given by

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m} + \sum_{\mathbf{R}_i} V_{\text{atom}}(\hat{\mathbf{r}} - \mathbf{R}_i) \\ &= \hat{H}_{\text{atom}, \mathbf{R}_j} + \Delta V_{\text{atom}, \mathbf{R}_j}(\hat{\mathbf{r}}) \end{aligned} \quad (94)$$

where we have defined

$$\Delta V_{\text{atom}, \mathbf{R}_j}(\mathbf{r}) := \sum_{\mathbf{R}_i \neq \mathbf{R}_j} V_{\text{atom}}(\mathbf{r} - \mathbf{R}_i) \quad (95)$$

as the perturbation of the \mathbf{R}_j atom potential due to the presence of all other atoms. Treating this as a small term is precisely the spirit of the tight-binding approximation.

We are thus lead to computing the matrix elements of the Hamiltonian in the eigenstates

of two atoms j and l in order to solve the perturbed problem

$$\langle \alpha, \mathbf{R}_j | \hat{H} | \beta, \mathbf{R}_l \rangle = \epsilon_\alpha \delta_{\alpha,\beta} \delta_{\mathbf{R}_j, \mathbf{R}_l} + \langle \alpha, \mathbf{R}_j | \Delta \hat{V}_{\text{atom}, \mathbf{R}_j} | \beta, \mathbf{R}_l \rangle. \quad (96)$$

The last term describes the tunneling of an electron in orbital α of atom j to orbital β of atom l . This is only likely to happen if \mathbf{R}_j and \mathbf{R}_l are close to one another.

In order to make progress, let us directly assume a form for these matrix elements. Let us focus on atoms placed on a simple square lattice in 2D with lattice constant a , $N_x \times N_y$ sites and periodic boundary conditions. We consider only the lowest s orbital of each atom. If we also neglect the electron spin degree of freedom (implicitly assuming that everything is trivially spin-degenerate), we can drop the index α on each atom. Now, set

$$\langle \mathbf{R}_j | \Delta \hat{V}_{\text{atom}, \mathbf{R}_j} | \mathbf{R}_l \rangle = \begin{cases} -t & \text{if } \mathbf{R}_j \text{ and } \mathbf{R}_l \text{ are nearest neighbors} \\ -t' & \text{if } \mathbf{R}_j \text{ and } \mathbf{R}_l \text{ are next-nearest neighbors} \\ 0 & \text{else.} \end{cases} \quad (97)$$

We also drop the irrelevant global shift of all onsite energies.

This is a great occasion to introduce second quantized notation, even though it is absolutely not needed for this problem. However, the hopping processes are intuitively understood in the second quantized language. We rewrite the tight-binding problem as

$$\hat{H}_{\text{tight-binding}} = -t \sum_{\langle \mathbf{R}_j, \mathbf{R}_l \rangle} c_{\mathbf{R}_j}^\dagger c_{\mathbf{R}_l} - t' \sum_{\langle\langle \mathbf{R}_j, \mathbf{R}_l \rangle\rangle} c_{\mathbf{R}_j}^\dagger c_{\mathbf{R}_l}, \quad (98)$$

where $c_{\mathbf{R}_j}^\dagger$ ($c_{\mathbf{R}_j}$) is the creation (annihilation) operator for an electron on site \mathbf{R}_j and the summation subscripts $\langle \mathbf{R}_j, \mathbf{R}_l \rangle$ ($\langle\langle \mathbf{R}_j, \mathbf{R}_l \rangle\rangle$) are frequently used to indicate sums over nearest (next-nearest) neighbors. Rewriting the second quantized operators using their Fourier transform

$$c_{\mathbf{R}_j}^\dagger = \frac{1}{\sqrt{N_x N_y}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_j} c_{\mathbf{k}}^\dagger, \quad (99)$$

where the sum is taken over the first BZ $\mathbf{k} = 2\pi/a(n/N_x, m/N_y)$, $n = 0, \dots, N_x - 1$, $m = 0, \dots, N_y - 1$, we obtain

$$\hat{H}_{\text{tight-binding}} = - \sum_{\mathbf{k}} \{ 2t [\cos(k_x a) + \cos(k_y a)] + 4t' [\cos(k_x a) \cos(k_y a)] \} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}. \quad (100)$$

We observe that the Hamiltonian is readily diagonal in momentum space so that we can read off the energy band dispersion

$$\begin{aligned}\epsilon_{\mathbf{k}} &= -2t[\cos(k_x a) + \cos(k_y a)] - 4t'[\cos(k_x a) \cos(k_y a)] \\ &= -4t - 4t' - \frac{\mathbf{k}^2}{2m^*} + \mathcal{O}(\mathbf{k}^4),\end{aligned}\tag{101}$$

where the effective mass $m^* = (2t + 8t')^{-1}$ near $\mathbf{k} = 0$. Expanding the Hamiltonian and energy bands in small deviations \mathbf{p} around a momentum point \mathbf{k} is called a $\mathbf{k} \cdot \mathbf{p}$ approximation.

D. Wannier states

The Fourier transform of Bloch wave functions

$$|\mathbf{R}, n\rangle = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}} |\mathbf{k}, n\rangle\tag{102}$$

is called a Wannier function and provides an alternative basis for the single particle Hilbert space, where n is a band index. It has the properties

$$W_n(\mathbf{r} - \mathbf{R}) \equiv \langle \mathbf{r} | \mathbf{R}, n \rangle,\tag{103}$$

i.e., it is a function of $(\mathbf{r} - \mathbf{R})$ only and

$$\begin{aligned}\int d\mathbf{r} W_n^*(\mathbf{r} - \mathbf{R}) W_m(\mathbf{r} - \mathbf{R}') &= \frac{1}{\Omega} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k} \cdot \mathbf{R} - \mathbf{k}' \cdot \mathbf{R}')} \int d\mathbf{r} \psi_{n, \mathbf{k}'}^*(\mathbf{r}) \psi_{m, \mathbf{k}}(\mathbf{r}) \\ &= \frac{1}{\Omega} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k} \cdot \mathbf{R} - \mathbf{k}' \cdot \mathbf{R}')} \delta_{\mathbf{k}, \mathbf{k}'} \delta_{n, m} \\ &= \delta_{\mathbf{R}, \mathbf{R}'} \delta_{n, m}.\end{aligned}\tag{104}$$

It is important to stress the role of a *gauge freedom* here. In momentum space, we can change the gauge of the Bloch states by multiplying with any momentum-dependent $U(1)$ phase factor $\varphi(\mathbf{k})$

$$|\mathbf{k}, n\rangle \rightarrow e^{i\varphi(\mathbf{k})} |\mathbf{k}, n\rangle.\tag{105}$$

This local transformation in momentum space has to leave all physical observables invariant. However, following Eq. (102) it changes the Wannier functions shape in real space, i.e., it changes the shape of the real space basis functions. In a multi-band system either a $U(1) \times \cdots \times U(1)$ gauge transformation or, for N degenerate bands, a $U(N)$ gauge transformation is allowed.

E. Interlude: Group representations and character tables

The group of symmetry operations of a crystal constrains the electronic structure in momentum space, as we shall see in the next section. To be prepared for this, we need to quickly learn or recall some facts about the representation of groups.

A *representation* of a group over some vector space V is a collection of linear operators on this vector space, which satisfy the same algebra as the group elements. As we are only concerned with finite groups, we can always think of these operators as matrices. An *irreducible representation* is a set of such matrix operators that is simultaneously block-diagonalized and cannot be diagonalized into smaller blocks anymore.

To be concrete and explicit, we will illustrate the terminology that is introduced using the example of the symmetry group of an equilateral triangle, C_{3v} (the latter is called the Schoenflies symbol for the group). The symmetry group consists of an identity element E , clockwise and anti-clockwise rotations by $\pm 2\pi/3$, denoted by C_3 and C_3^2 , as well as reflections σ_v , σ'_v , and σ''_v that exchange a pair of corners each. We now represent these operations on $V = \mathbb{R}^3$ as

$$\begin{aligned} E &= \mathbb{1}_{3 \times 3}, & C_3 &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, & C_3^2 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\ \sigma_v &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, & \sigma'_v &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & \sigma''_v &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{106}$$

If the three components of the vector in V represent the corners of the triangle (A, B, C) , then we directly see that for instance $C_3(A, B, C)^\top = (B, C, A)^\top$ implements the desired rotation (cyclic permutation).

The above representation of the symmetry group is reducible. To see that, we perform the similarity transformation

$$R = \begin{pmatrix} 1/\sqrt{3} & 2/\sqrt{6} & 0 \\ 1/\sqrt{3} & -1/\sqrt{6} & 1/\sqrt{2} \\ 1/\sqrt{3} & -1/\sqrt{6} & -1/\sqrt{2} \end{pmatrix}, \tag{107}$$

which brings any of $G \in \{E, C_3, C_3^2, \sigma_v, \sigma'_v, \sigma''_v\}$ to a block-diagonal form $\tilde{G} = R^{-1}GR$.

Concretely

$$\begin{aligned}
\tilde{E} &= \mathbb{1}_{3 \times 3}, & \tilde{C}_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, & \tilde{C}_3^2 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
\tilde{\sigma}_v &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, & \tilde{\sigma}'_v &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, & \tilde{\sigma}''_v &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}.
\end{aligned} \tag{108}$$

We have managed to split up the representation of the group into two irreducible representations, one with dimension one and one with dimension two. Information about the irreducible representations is summarized in *character tables*.

C_{3v}	E	C_3	C_3^2	σ_v	σ'_v	σ''_v
A_1	1	1	1	1	1	1
E	2	-1	-1	0	0	0

The entries of the table (the characters) are the trace of the respective irreducible representation. Group element representations of the same class have the same trace and are thus usually summarized in a character table. We also note that we have not discovered one more irreducible representations via our considerations, which corresponds to rotations in three-dimensional space. The full character table of C_{3v} thus reads as follows

C_{3v}	E	$2C_3$	$3\sigma_v$	basis functions
A_1	1	1	1	$z, x^2 + y^2, z^2$
A_2	1	1	-1	R_z
E	2	-1	0	$(x, y), (R_x, R_y), (x^2 - y^2, xy), (xz, yz)$

The first column consists of the Mulliken symbols of the irreducible representations and we have added the basis functions to lowest power in the coordinates in the last column. These basis functions transform under the symmetry operations as the irreducible transformations do. Note that the entry in the column E that corresponds to the identity element of the group always gives the dimension of the irreducible representation. The number of classes of group elements is always equal to the number of irreducible representations. There are various further constraints on the entries of the character table. For example, the sum of the

squares of the dimensions of the irreducible representations equals the order of the group (i.e., the number of group elements).

The characters also contain information about how the irreducible representations transform under the symmetry operations. In groups that contain inversion, the subscript ‘u’ and ‘g’ with the Mulliken symbol stands for even and odd irreducible basis functions under inversion.

Below we will need the character tables for the groups O_h and D_{4h} which are given in Fig. 3.

Character table for O_h point group												
	E	$8C_3$	$6C_2$	$6C_4$	$3C_2=(C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	linear, rotations	quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xz, yz, xy)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

Character table for D_{4h} point group												
	E	$2C_4(z)$	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linear, rotations	quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x, y)	

Figure 3. Character tables for the point groups O_h and for D_{4h} , which is a subgroup of the former.

F. Symmetries in band structures

We have already explored the symmetries of crystal lattices and the implications for functions defined on such a lattice. It is now imperative to ask how this carries over to quantum-mechanical band structures and Bloch states.

Let $S_{\{g,\mathbf{a}\}}$ be the representation of an element of the space group when acting on a wave function

$$S_{\{g,\mathbf{a}\}}\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\{g,\mathbf{a}\}^{-1}\mathbf{r}) = \psi_{\mathbf{k}}(g^{-1}\mathbf{r} - g^{-1}\mathbf{a}) \quad (109)$$

where the inverse appears because $\hat{S}_{\{g,\mathbf{a}\}}|\mathbf{r}\rangle = |g\mathbf{r} + \mathbf{a}\rangle$, but $\langle\mathbf{r}|\hat{S}_{\{g,\mathbf{a}\}} = \langle g^{-1}\mathbf{r} - g^{-1}\mathbf{a}|$. We now show that the transformed wave function $\psi_{\mathbf{k}}(g^{-1}\mathbf{r} - g^{-1}\mathbf{a})$ is also an eigenstate of the translation operator

$$\begin{aligned} T_{\mathbf{a}'}S_{\{g,\mathbf{a}\}}\psi_{\mathbf{k}}(\mathbf{r}) &= S_{\{g,\mathbf{a}\}}T_{g^{-1}\mathbf{a}'}\psi_{\mathbf{k}}(\mathbf{r}) \\ &= S_{\{g,\mathbf{a}\}}e^{-i\mathbf{k}\cdot(g^{-1}\mathbf{a}')} \psi_{\mathbf{k}}(\mathbf{r}) \\ &= e^{-i(g\mathbf{k})\cdot\mathbf{a}'} S_{\{g,\mathbf{a}\}}\psi_{\mathbf{k}}(\mathbf{r}), \end{aligned} \quad (110)$$

but with an eigenvalue determined by $g\mathbf{k}$ rather than \mathbf{k} . This suggests that $\psi_{\mathbf{k}}(g^{-1}\mathbf{r} - g^{-1}\mathbf{a})$ is (proportional to) $\psi_{g\mathbf{k}}(\mathbf{r})$. Indeed, because the Bloch wave functions have the periodicity of the lattice $S_{\{g,\mathbf{a}\}}u_{\mathbf{k}}(\mathbf{r}) = u_{g\mathbf{k}}(\mathbf{r})$ we have

$$\begin{aligned} S_{\{g,\mathbf{a}\}}\psi_{\mathbf{k}}(\mathbf{r}) &= \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot(g^{-1}\mathbf{r} - g^{-1}\mathbf{a})} u_{g\mathbf{k}}(\mathbf{r}) \\ &= e^{-i(g\mathbf{k})\cdot\mathbf{a}} \psi_{g\mathbf{k}}(\mathbf{r}). \end{aligned} \quad (111)$$

From this transformation property, we can infer, for example, the symmetries of the band structure

$$\epsilon_{\mathbf{k}} = \langle\mathbf{k}|\hat{H}|\mathbf{k}\rangle = \langle\mathbf{k}|\hat{S}_{\{g,\mathbf{a}\}}^{-1}\hat{H}\hat{S}_{\{g,\mathbf{a}\}}|\mathbf{k}\rangle = \langle g\mathbf{k}|\hat{H}|g\mathbf{k}\rangle = \epsilon_{g\mathbf{k}}, \quad (112)$$

which defines a ‘star’ of \mathbf{k} points whose band eigenvalues are related.

Notice that the above calculation assumed nondegenerate bands. If the bands are degenerate then $\hat{S}_{\{g,\mathbf{a}\}}$ may also act nontrivially on this internal degree of freedom. The action that leaves \mathbf{k} unchanged is the aforementioned little group symmetry of \mathbf{k} . Assume that we have a set of d degenerate states at some momentum

$$\hat{H}|n, \mathbf{k}\rangle = \epsilon_{\mathbf{k}}|n, \mathbf{k}\rangle, \quad n = 1, \dots, d. \quad (113)$$

For every element of the little group of \mathbf{k} , $\hat{S}_{\{g|\mathbf{a}\}}$ we have a representation of the symmetry

$$\hat{S}_{\{g|\mathbf{a}\}}|n, \mathbf{k}\rangle = \sum_{n'} |n', \mathbf{k}\rangle M_{n,n';\mathbf{k}}, \quad M_{n,n';\mathbf{k}} = \langle n', \mathbf{k} | \hat{S}_{\{g|\mathbf{a}\}} | n, \mathbf{k} \rangle. \quad (114)$$

If the representation is irreducible, its dimension is that of the Bloch states at the momentum \mathbf{k} .

Example: Consider a tight-binding model for p -orbitals on a cubic lattice spanned by the basis vectors \mathbf{a}_x , \mathbf{a}_y , and \mathbf{a}_z . On each lattice site there are three atomic orbitals with the from

$$\begin{aligned} \langle \mathbf{r} | x, \mathbf{R} \rangle &= (\mathbf{R} - \mathbf{r})_x f(|\mathbf{R} - \mathbf{r}|), \\ \langle \mathbf{r} | y, \mathbf{R} \rangle &= (\mathbf{R} - \mathbf{r})_y f(|\mathbf{R} - \mathbf{r}|), \\ \langle \mathbf{r} | z, \mathbf{R} \rangle &= (\mathbf{R} - \mathbf{r})_z f(|\mathbf{R} - \mathbf{r}|), \end{aligned} \quad (115)$$

which due to the symmetry of the simple cubic lattice remain degenerate in energy. For nearest neighbors, the overlaps from Eq. (96) evaluate to

$$\langle \alpha, \mathbf{R}_j | \Delta \hat{V}_{\text{atom}, \mathbf{R}_j} | \beta, \mathbf{R}_j + \mathbf{a}_\gamma \rangle = \begin{cases} t\delta_{\alpha,\beta} & \text{for } \gamma = \alpha \quad \sigma\text{-bonding} \\ -\tilde{t}\delta_{\alpha,\beta} & \text{for } \gamma \neq \alpha \quad \pi\text{-bonding,} \end{cases} \quad (116)$$

with $\alpha, \beta, \gamma \in \{x, y, z\}$. For next-nearest neighbors, the overlaps from Eq. (96) evaluate to (for $\gamma \neq \rho$)

$$\langle \alpha, \mathbf{R}_j | \Delta \hat{V}_{\text{atom}, \mathbf{R}_j} | \beta, \mathbf{R}_j + \mathbf{a}_\gamma \pm \mathbf{a}_\rho \rangle = \begin{cases} t'\delta_{\alpha,\beta} & \text{for } \gamma = \alpha \\ -\tilde{t}'\delta_{\alpha,\beta} & \text{for } \gamma \neq \alpha \\ -(\pm)\tilde{t}'\delta_{\alpha,\gamma}\delta_{\beta,\sigma} & \end{cases} \quad (117)$$

with $\alpha, \beta, \gamma \in \{x, y, z\}$. Notice that some hoppings are zero by symmetry, for example the hopping along the x direction from an x to a y orbital.

Translating the above into a second quantized Hamiltonian in momentum space yields (we set the lattice constant to unity)

$$\hat{H}_p = \sum_{\mathbf{k}} (c_{p_x, \mathbf{k}}^\dagger, c_{p_y, \mathbf{k}}^\dagger, c_{p_z, \mathbf{k}}^\dagger) \begin{pmatrix} E_x(\mathbf{k}) & -4\tilde{t}' \sin k_x \sin k_y & -4\tilde{t}' \sin k_x \sin k_z \\ -4\tilde{t}' \sin k_x \sin k_y & E_y(\mathbf{k}) & -4\tilde{t}' \sin k_y \sin k_z \\ -4\tilde{t}' \sin k_x \sin k_y & -4\tilde{t}' \sin k_y \sin k_z & E_z(\mathbf{k}) \end{pmatrix} \begin{pmatrix} c_{p_x, \mathbf{k}} \\ c_{p_y, \mathbf{k}} \\ c_{p_z, \mathbf{k}} \end{pmatrix} \quad (118)$$

with

$$E_x(\mathbf{k}) = 2t \cos k_x - 2\tilde{t}(\cos k_y + \cos k_z) + 4t' \cos k_x (\cos k_y + \cos k_z) - 4\tilde{t}' \cos k_y \cos k_z, \quad (119)$$

and the analogous expressions for $E_y(\mathbf{k})$ and $E_z(\mathbf{k})$. We have neglected an overall on-site energy shift which is equal for all p -orbitals.

We can now analyze the degeneracies of this band structure at high-symmetry points. At the Γ point, $\mathbf{k} = 0$, we have the full crystal symmetry of the O_h group, the Bloch matrix simplifies to

$$(2t + 8t' - 4\tilde{t} - 4\tilde{t}')\mathbb{1}_{3 \times 3}, \quad (120)$$

and accordingly all three bands are degenerate belonging to the representation T_{1u} of O_h . At the X point, $\mathbf{k} = (0, 0, \pi)$, the little group is D_{4h} (a tetragonal symmetry) and the Bloch matrix is given by

$$\text{diag}(-2t - 8t' - 4\tilde{t} - 4\tilde{t}', 2t + 4\tilde{t}', 2t + 4\tilde{t}'), \quad (121)$$

which is separated into a two-fold degenerate irreducible representation $[E_u]$, corresponding to basis functions (x, y) and a singly degenerate one $[A_{2u}]$, corresponding to basis function z .

G. Filling of bands and density of states

So far we have only considered a single particle picture of electronic bands. In a many-body Hilbert space, fermionic states can all be at most singly occupied. In the ground state at zero temperature, all states below the *Fermi level* in a solid are singly occupied, all states above are empty. The occupied states form the *Fermi sea*. If the Fermi level is located such that it cuts through a band (or more generally, there are excited states at arbitrarily low energy available) one speaks of a metal. For a noninteracting system, the locations in momentum space of these single-particle excitations with arbitrary low energy and momentum transfer, form the *Fermi surface*. Materials with a finite excitation energy above the ground state are called semiconductors (for small excitation energies) or insulators (for large excitation energies). At finite temperature, the single-particle levels dictated by the band structure are occupied according to the Fermi-Dirac distribution.

When counting the number of states available, it is always important to pay attention whether spin-degeneracies have to be taken into account or not. If all bands are spin degen-

erate (as is the case in an electronic model which neglects spin-orbit and Zeeman couplings), each state can be occupied by a spin-up and a spin-down electron.

To better understand the relation between the band dispersion and the number of occupied states, we return to the example of the simple square lattice and restrict it to nearest neighbor hopping only. The dispersion is $\epsilon_{\mathbf{k}} = -2t \cos k_x - 2t \cos k_y$. We want to compute the density of states, i.e., $dN/d\epsilon$, where N is the number of occupied states. One interesting point is the band bottom and the zero energy around which $\epsilon_{\mathbf{k}} \approx \mathbf{k}^2/(2m^*)$. We have in 2D $dN = 2\pi k dk$ and $k = \sqrt{2m^*\epsilon}$ such that

$$\frac{dN}{d\epsilon} = \frac{dN}{dk} \frac{dk}{d\epsilon} = 2\pi k \sqrt{\frac{m^*}{2\epsilon}} = 2\pi m^*, \quad (122)$$

i.e., it is a constant. The same calculation yields in 1D $dN/d\epsilon \propto 1/\sqrt{\epsilon}$ and in 3D $dN/d\epsilon \propto \sqrt{\epsilon}$. The second interesting point to consider in 2D is near $\mathbf{k} = (\pi, 0)$ and symmetry equivalent. The effective band dispersion is $\epsilon_{\mathbf{k}} \approx (k_y^2 - k_x^2)/(2m^*)$, i.e., it is a saddle point. The density of states is given by

$$\begin{aligned} \frac{dN}{d\epsilon} &\propto \int dk_x dk_y \delta[\epsilon - (k_y^2 - k_x^2)/(2m^*)] \\ &\propto \int dk_x \frac{1}{\sqrt{2m^*\epsilon + k_x^2}} \\ &\propto \log \left[k_x + \sqrt{k_x^2 + 2m^*\epsilon} \right] \Big|_0^\Lambda \\ &\propto (\text{regular part}) - \log \epsilon, \end{aligned} \quad (123)$$

i.e., we find a log divergence as the energy approaches the saddle point in 2D. This is called a van Hove singularity. [See Fig. 2 b).]

H. Coupling to an external electro-magnetic field

Electrons couple to a magnetic field in two ways which are considered distinct in the realm of condensed matter physics (of course they are unified on the level of relativistic quantum mechanics): For one due to their orbital motion to the electromagnetic gauge field and on the other hand due to the Zeeman effect to the electronic spin. The former can be accounted for by minimal coupling, i.e., the replacement

$$\hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) \rightarrow \hat{H}(\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{r}}), \hat{\mathbf{r}}). \quad (124)$$

The latter is an additive term

$$\hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) \rightarrow \hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{r}}) + \mu_B g^* \hat{\mathbf{S}} \cdot \mathbf{B}, \quad (125)$$

where $\hat{\mathbf{S}}$ is the spin operator and g^* is the effective Landé g factor, which is $g = 2$ for the free electron but can deviate substantially in the electronic environment of crystals, where values of $g^* = 20$ are easily possible. Depending on the physics one is interested in, often only one of the two effects is considered at a time. Typically, the orbital coupling has the more dramatic effect on the electronic structure and we will explore its consequences in the following sections.

1. Semiclassical equations of motion

A minimal way to include quantum-mechanical phenomena in the description of electrons in solids is to consider the dynamics of wave packets which are extended both in position and momentum space. We write a wave function of the form

$$\psi_{\mathbf{k}}(\mathbf{r}, t) = \sum_{\mathbf{k}'} g_{\mathbf{k}}(\mathbf{k}') e^{i\mathbf{k}' \cdot \mathbf{r} - i\epsilon_{\mathbf{k}'} t}, \quad (126)$$

where $g_{\mathbf{k}}(\mathbf{k}')$ is a function centered around \mathbf{k} with a characteristic width Δk much smaller than the size of the BZ. In turn, by the uncertainty principle the wave packet $\psi_{\mathbf{k}}(\mathbf{r}, t)$ is spread over many unit cells in position space. Assuming that the system is perturbed weakly by electric and magnetic fields, \mathbf{E} and \mathbf{B} , such that no interband transitions are induced, one can derive the following equations of motion

$$\begin{aligned} \dot{\mathbf{r}} &\equiv \mathbf{v}_n(\mathbf{k}) = \frac{\partial \epsilon_{n,\mathbf{k}}}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}) \\ \dot{\mathbf{k}} &= -e\mathbf{E}(\mathbf{r}, t) - e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r}, t). \end{aligned} \quad (127)$$

Notice that \mathbf{k} is the pseudo momentum of the electron (i.e., related to the expectation value of the translation operator), not the expectation value of the momentum operator. The quantity $\boldsymbol{\Omega}_n(\mathbf{k})$ is a purely quantum-mechanical contribution known as the Berry curvature. From the Bloch eigenstates of the bands, it is defined as

$$\Omega_{n,\alpha}(\mathbf{k}) = -\epsilon_{\alpha,\beta,\gamma} i \langle \partial_{k_\beta} u_{n,\mathbf{k}} | \partial_{k_\gamma} u_{n,\mathbf{k}} \rangle. \quad (128)$$

From the form of Eq. (127) it is suggestive to interpret the Berry curvature as a 'magnetic field in momentum space', that has physical consequences for the electron motion in position space.

Let us consider a 1D system with dispersion $\epsilon_k = -2 \cos k$ in a static electric field E . Equation (127) reads for this case

$$\dot{x} = 2 \sin k, \quad \dot{k} = -eE, \quad \Rightarrow \quad \dot{x} = -2 \sin(eEt) \quad (129)$$

thus, the position of the wave packet oscillates according to

$$x(t) = \frac{2}{eE} \cos(eEt), \quad (130)$$

which are called *Bloch oscillations*. They can be observed in very clean systems.

Now, consider a system which for simplicity is taken to have a quadratic band dispersion (such that $\partial \epsilon_{n,\mathbf{k}} \partial \mathbf{k} = \mathbf{k}/m$) with applied homogeneous electric field \mathbf{E} . We study two situations (1) with an applied external homogeneous magnetic field \mathbf{B} and (2) with a nonvanishing intrinsic Berry curvature $\mathbf{\Omega}$.

For (1), the equations of motion reduce to

$$m\dot{\mathbf{v}} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (131)$$

We are interested in steady state solutions $\dot{\mathbf{v}} = 0$, i.e.,

$$\mathbf{v} \times \mathbf{B} = -\mathbf{E}. \quad (132)$$

The electric current is $\mathbf{j} = -en_0\mathbf{v}$, where n_0 is the carrier density. Comparing the above to the definition of the conductivity $j_\alpha = \sigma_{\alpha,\beta}E_\beta$, we find that the system has a non-vanishing *Hall response*. Taking $\mathbf{B} = (0, 0, B_z)$ and $\mathbf{E} = (E_x, 0, 0)$, we have

$$\sigma_{xy} = j_y/E_x = n_0e/B_z = \nu e^2/h, \quad (133)$$

where $\nu = n_0hc/(Be)$ is called the filling fraction and we have reinstated the appropriate factors of c and h to obtain the well known form of the Hall conductivity. Measuring the Hall response can thus determine both the carrier density and the electron or hole like nature of the carriers.

For (2) we find

$$\mathbf{v} = \frac{\mathbf{k}}{m} + e\mathbf{E} \times \mathbf{\Omega}, \quad (134)$$

i.e., the Berry connection induces a Hall response similar to an external magnetic field. For a 2D system in the x - y plane with only one (partially) filled band the area of the Fermi sea S_{FS} is the density of carriers n_0 . Taking the latter to be $(2\pi)^2$, we find

$$\mathbf{j} = \frac{e^2}{h/(2\pi)} S_{\text{FS}} \left[\int_{\text{FS}} \frac{d^2\mathbf{k}}{(2\pi)^2} \mathbf{\Omega}(\mathbf{k}) \right] \times \mathbf{E}, \quad (135)$$

where the integral is taken over the Fermi sea (FS). Thus, the Hall conductivity for such a system is given by

$$\sigma_{xy} = \frac{e^2}{h} 2\pi \frac{S_{\text{FS}}}{(2\pi)^2} \int_{\text{FS}} d^2\mathbf{k} \Omega_z(\mathbf{k}). \quad (136)$$

Notice that if the band is completely filled, i.e., the system is an insulator $S_{\text{FS}} = (2\pi)^2$ and the Hall response can still be nonzero. In fact, it is then given by $e^2/h 2\pi \int d^2\mathbf{k} \Omega_z(\mathbf{k})$, which for deep mathematical reasons is always an integer called the Chern number.

2. The integer quantum Hall effect

Quantum Hall effects are one of the driving thrusts of condensed matter research of the past decades. Here, we will first consider the integer quantum Hall effect (IQHE) which can be understood without considering electron-electron interactions. Later, we will mention the fractional quantum Hall effect (FQHE), which needs interactions to exist.

The possibility of an IQHE was first noted in a theoretical paper by Ando et al. in 1975, but the authors doubted that their result connects to the realm of experiments. The Nobel-prize winning experimental discovery of the IQHE by von Klitzing et al. thus came as a big surprise. In the experimental setup, electrons of charge $e < 0$ and effective mass m are confined to a 2D plane in a high-quality GaAs heterojunction and a large magnetic field B is applied perpendicular to that plane. In this situation, the electronic density of states consists of discrete peaks, the so-called Landau levels. These Landau level bands are broadened by disorder and equally spaced in energy with spacing given by the cyclotron frequency $\omega_c := eB/m$. If the broadening is small enough such that there exist insulating regions between the peaks, the transverse conductivity σ_H is quantized in units of the resistance quantum e^2/h whenever the chemical potential lies within such an insulating region. One year after the experimental discovery, Laughlin gave a theoretical explanation for the high-precision quantization of the conductivity. However, his description did not account for the topological nature of the IQHE. The deep connection to topological quantum numbers was made one year later by Thouless, Kohmoto, Nightingale, and den Nijs (TKKN).

The completion of the theoretical understanding of the IQHE coincided with the next groundbreaking and Nobel-prize winning experimental discovery made by Störmer, Tsui and coworkers in 1982. They observed that plateaus in the Hall resistance develop at fractional fillings ν of the Landau level, accompanied by a dip or vanishing of the longitudinal resis-

tance. This FQHE turned out to have a much richer phenomenology than the integer effect with more and more examples of stable filling fractions discovered as the sample quality improved. As with the IQHE, it was Laughlin who gave a theoretical explanation for the occurrence of the principal filling fractions $\nu = 1/n$, $n \in \mathbb{Z}$, based on the specific form of the quantum state of the two-dimensional electron gas. However, he did not make the connection to the topological character of the state which was later established by Wen and Niu.

We consider a 2D electron gas in the x - y plane in a magnetic field $\mathbf{B} = (0, 0, -B)$ that is orbitally coupled to the motion of the electrons. Such a situation can occur in heterostructure interfaces. We have

$$\hat{H} = \frac{1}{2m} [(\hat{p}_x - eA_x(\hat{\mathbf{r}}))^2 + (\hat{p}_y - eA_y(\hat{\mathbf{r}}))^2], \quad (137)$$

where m is not necessarily the bare electron mass, but an effective mass. We now introduce the operators

$$\hat{a}^\dagger = \frac{\ell}{\sqrt{2}} [(\hat{p}_x - eA_x(\hat{\mathbf{r}})) + i(\hat{p}_y - eA_y(\hat{\mathbf{r}}))], \quad \hat{a} = \frac{\ell}{\sqrt{2}} [(\hat{p}_x - eA_x(\hat{\mathbf{r}})) - i(\hat{p}_y - eA_y(\hat{\mathbf{r}}))], \quad (138)$$

where $\ell^2 = (eB)^{-1}$ is the magnetic length. Their algebra

$$\begin{aligned} \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} &= -\frac{i\ell^2 e}{2} ([\hat{p}_x, A_y(\hat{\mathbf{r}})] - [\hat{p}_y, A_x(\hat{\mathbf{r}})]) + \frac{i\ell^2 e}{2} ([\hat{p}_y, A_x(\hat{\mathbf{r}})] - [\hat{p}_x, A_y(\hat{\mathbf{r}})]) \\ &= \frac{\ell^2 e}{2} (\partial_y A_x(\mathbf{r}) - \partial_x A_y(\mathbf{r})) - \frac{\ell^2 e}{2} (\partial_x A_y(\mathbf{r}) - \partial_y A_x(\mathbf{r})) \\ &= \ell^2 e B \\ &= 1 \end{aligned} \quad (139)$$

allows them to be interpreted as bosonic lowering and raising operators. We can define a second set of operators

$$\begin{aligned} \hat{b}^\dagger &= \frac{1}{\sqrt{2}\ell} \left\{ \hat{r}_x - \ell^2(\hat{p}_y - e\hat{A}_y) + i[\hat{r}_y + \ell^2(\hat{p}_x - e\hat{A}_x)] \right\}, \\ \hat{b} &= \frac{1}{\sqrt{2}\ell} \left\{ \hat{r}_x - \ell^2(\hat{p}_y - e\hat{A}_y) - i[\hat{r}_y + \ell^2(\hat{p}_x - e\hat{A}_x)] \right\}, \end{aligned} \quad (140)$$

which realize an independent bosonic algebra for

$$[\hat{a}, \hat{b}] = 0, \quad [\hat{a}, \hat{b}^\dagger] = 0, \quad [\hat{b}, \hat{b}^\dagger] = 1. \quad (141)$$

The Hamiltonian rewritten in terms of these operators reads

$$\hat{H} = \omega_c \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right). \quad (142)$$

where again $\omega_c = eB/m$ is the cyclotron frequency. The energy spectrum is that of a harmonic oscillator, $E_n = \omega_c(n + 1/2)$, $n = 0, 1, 2, \dots$. Each of these energy levels is called *Landau level*. However, due to the commuting operator b , every level is highly degenerate, as its single-particle eigenstates can be written $|n, m\rangle = (n!m!)^{-1/2} \hat{a}^\dagger{}^n \hat{b}^\dagger{}^m |0\rangle$. To understand this better, consider the eigenstates of the lowest Landau level in a symmetric gauge $\mathbf{A} = (-Br_y, Br_x, 0)/2$

$$\langle \mathbf{r} | 0, m \rangle = \frac{1}{\sqrt{2\pi 2^m m!} \ell} \left(\frac{z}{\ell} \right)^m e^{-|z|^2/(4\ell^2)}, \quad m = 0, 1, 2, \dots, \quad (143)$$

where $z = r_x - ir_y$. We have $\langle 0, m | \hat{\mathbf{r}}^2 | 0, m \rangle = 2(m + 1)\ell^2$. The amplitude of the wave function $\langle \mathbf{r} | 0, m \rangle$ is peaked at a radius $r_m = \sqrt{2m}\ell$. This means that the area taken by a ‘‘Hall droplet’’ with all states $m < m_0$ filled, is proportional to m_0 and the inverse field strength. Thus the Landau level degeneracy m_0 is given by the area S of the system divided by the area taken by one magnetic flux quantum $m_0 \sim S/(2\pi\ell^2)$. (The magnetic flux quantum is $\Phi_0 = hc/e$.)

To study the transport response, it is easier to use the Landau gauge $\mathbf{A} = (0, Br_x, 0)$. Then, k_y is a good quantum number (instead of the angular momentum in the case of the symmetric gauge) and

$$\psi_{0, k_y} = \frac{1}{\sqrt{2\pi}\ell} e^{-[r_x - x_0(k_y)]^2/(2\ell^2)} e^{ik_y r_y}, \quad (144)$$

with $x_0(k_y) = \ell^2 k_y$, are the lowest Landau level wave functions. The energy is independent of k_y . We now apply an electric field E_x in x -direction, which enters the Hamiltonian as the additive term $-eE_x \hat{r}_x$. Clearly, this term can be absorbed by shifting the origin of the x axis, which amounts to the replacement $x_0(k_y) \rightarrow x'_0(k_y) := \ell^2 k_y + eE_x/(m\omega_c^2)$. However, the Landau level degeneracy is now lifted by the extra term such that the energies corresponding to the eigenstates ψ'_{0, k_y} read [see Fig. 4 a)]

$$E_0(k_y) = \frac{\omega_c}{2} - eE_x x'_0(k_y) + \frac{m^2}{2} \left(\frac{E_x}{B} \right)^2, \quad (145)$$

which allows us to directly read off the velocity

$$v_y(k_y) = \frac{dE_0(k_y)}{dk_y} = -E_x/B. \quad (146)$$

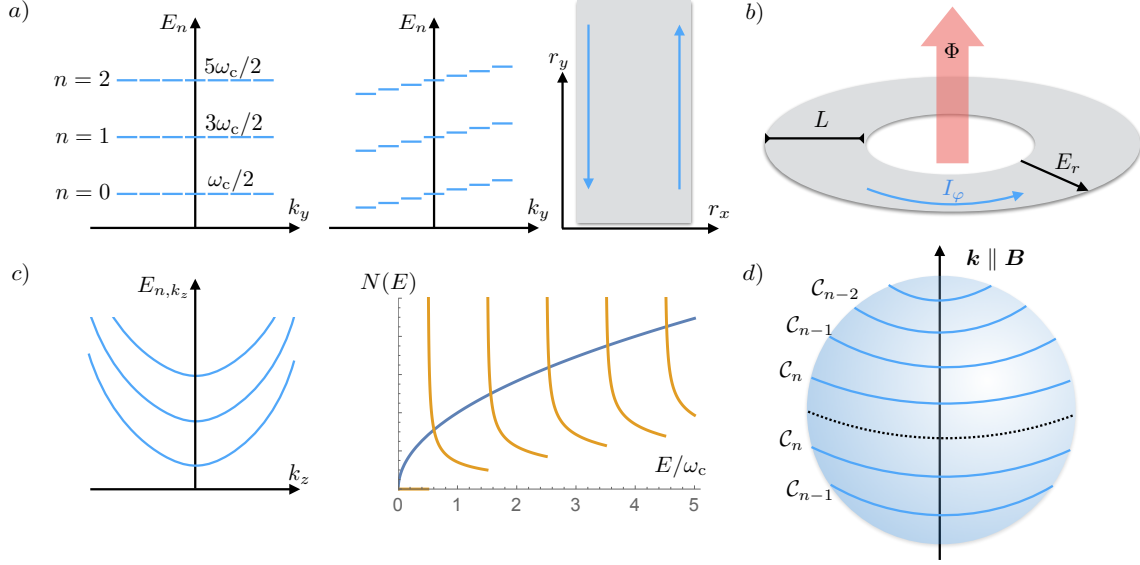


Figure 4. a) Landau level spectrum of a 2D electron gas without and with a linear potential in the x direction. The dispersion of the eigenstates in presence of the potential can be interpreted as an edge state propagating unidirectional at the sample boundary. b) Corbino disk geometry for Laughlin's flux insertion argument. c) Landau level band structure of a 3D electron gas and its density of states without (blue) and with magnetic field (orange). d) 3D Fermi sphere with extremal circle (dotted) and allowed semiclassical trajectories (blue lines) that are enclosed by wave packets in presence of a magnetic field.

There follows the Hall conductivity as

$$\sigma_{xy} = \nu \frac{e^2}{h}, \quad \nu = n_0 2\pi \ell^2. \quad (147)$$

a. Hall plateaus and disorder Von Klitzing's experimental observation was that the longitudinal conductivity σ_{yy} vanished for certain ranges of the magnetic field, which precisely corresponded to integer fillings $\nu \in \mathbb{N}$. At the same time, the Hall conductivity is quantized very precisely to the integer multiple of e^2/h that corresponds to the number of filled Landau levels. What was observed, however, is that the quantization forms stable plateaus over a full range of magnetic fields, not only for the exact field value that corresponds to a specific filling. This behavior can only be explained by considering the role of disorder in the system. For simplicity, we return to the symmetric gauge and add a rotationally symmetric disorder potential to the system of the form $V(\mathbf{r}) = C\mathbf{r}^2$. Its effect can be absorbed in the wave function (143) by replacing ℓ with $\ell' = \ell(1 + 2mC)^{-1/4}$. The Landau

level degeneracy is now lifted to

$$E_{0,m} = \frac{\omega_c}{2} \left[m \left(\frac{\ell^2}{\ell'^2} - 1 \right) + \frac{\ell^2}{\ell'^2} \right], \quad (148)$$

which for $m \gg 1$ and a weak potential $2mC \ll 1$ can be recast as

$$E_{0,m} \approx \frac{\omega_c}{2} + Cr_m^2, \quad (149)$$

where $r_m = \sqrt{2m}\ell'$ is the wave function localization radius. The locking between the wave function localization and the equipotential lines means that the quasiclassical trajectories trace out equipotential lines. A weak electric field cannot induce a motion of these wave packets in the orthogonal direction to the concentric rings. This picture can be elevated to a completely disordered sample as follows: At a specific chemical potential, equipotential lines that form a closed loop enclose states that do not contribute to bulk longitudinal transport. Only at specific values of the chemical potential, where the equipotential lines connect to form a delocalized channel that spans over the entire sample, connecting two leads, bulk transport can happen. Thus, when slightly doping away from the chemical potential corresponding to a filled Landau level, only small disconnected islands of equipotential lines appear and no transport is possible. The sample remains insulating and we observe a plateau in the Hall conductivity.

b. Edge states We now return to Eq. (145), namely the spectrum with an applied electric field in the x direction. This mathematical result allows for a second very different physical interpretation. For that, we reinterpret the source for the additional term in the Hamiltonian as being a (linear) confining potential at the sample boundary [see Fig. 4 a)]. We are then lead to the conclusion that the sample boundary hosts a set of states ψ_{0,k_y} with linear and unidirectional dispersion $E_{0,k_y} \propto k_y$ that propagate along the boundary. The fact that these modes can only move in one direction is very specific to the quantum Hall effect and cannot be realized in a system confined to strictly one dimension (a 1D systems hosts always as many right-moving modes as left-moving ones). While the velocity of these modes is not universal, the number of them (each filled Landau level contributed one branch of boundary modes) is in equal to the integer that determines the bulk Hall conductivity.

c. Laughlin's argument Laughlin gave an argument as to why the Hall conductivity of an insulator has to be quantized. The 2D insulator that is to be probed has the shape of a so-called Corbino disk, that is, a disk with a hole [see Fig. 4 b)]. The magnetic flux Φ trough

the center of the disk is varied in time. This flux does not change the field distribution in the disk and can therefore only be seen by states that extend fully around the disk. A change in the flux by $\delta\Phi$ can be accounted for by a change in the φ component of the vector potential $A_\varphi \rightarrow A_\varphi + \delta\Phi/(2\pi r)$. The symmetric gauge wave function (143) changes by $\psi_{0,m} \rightarrow \psi_{0,m} e^{i\varphi \delta\Phi/\Phi_0}$. This change can be absorbed by $m \rightarrow m - \delta\Phi/\Phi_0$. Hence, when increasing Φ by one flux quantum, the index m has to be decreased by 1. This implies that the wave functions are all continuously shifted in their localization radius during the flux insertion. As a result, one electron is pumped from the outer to the inner edge of the system after one flux quantum insertion.

When an electric field E_r is applied radially, the charge transfer results in a potential energy change $-eE_r L$, where L is the distance between the two edges of the disk, which we assume to be much smaller than the inner radius. A second energy change $I_\varphi \delta\Phi$ results from the current I_φ that is caused by the difference in angular momentum between the electronic states that were filled and emptied, respectively. After insertion of a full flux quantum, the energy of the system should remain unchanged, and hence these two energetic contributions must add up to zero. This leads to the relation $eE_r L = I_\varphi \Phi_0$. Returning to cartesian coordinates and reinstating all constants we obtain the Hall conductivity

$$\sigma_{xy} = \frac{j_y}{E_x} = \frac{I_y}{LE_x} = \frac{e^2}{h}. \quad (150)$$

This argument is topological in nature and thus valid independently for any Landau level and also for disordered systems.

3. Quantum oscillations

In studying the quantum Hall effect, we considered for simplicity a dispersion $\mathbf{p}^2/(2m)$ and introduced the magnetic field by minimal substitution. For other effective 2D dispersions, a similar Landau level structure emerges, where the energies of the degenerate Landau levels depend on the dispersion. For example, a linear dispersion as found around the K point in graphene leads to Landau level energies $\propto \sqrt{n}$.

Now, we want to extend the problem to a translationally invariant 3D systems in a homogeneous magnetic field, which we choose without loss of generality $\mathbf{B} = (0, 0, B)$. Working again the Landau gauge $\mathbf{A} = (0, Br_x, 0)$, the system retains its translational invariance along

the z direction even in presence of the magnetic field. It can thus be seen as a collection of 2D Landau level problems parametrized by the good quantum number k_z . The Hamiltonian

$$\hat{H} = \frac{[\hat{\mathbf{k}} - e\mathbf{A}(\hat{\mathbf{r}})]^2}{2m}, \quad (151)$$

has eigen wave functions

$$\psi_{n,k_y,k_z}(\mathbf{r}) = \frac{1}{\sqrt{2^n n! 2\pi \ell^2}} e^{ik_y r_y} e^{ik_z r_z} H_n[(r_x - k_y \ell^2)/\ell] e^{-(r_x - k_y \ell^2)^2/(2\ell^2)} \quad (152)$$

with energies

$$E_{n,k_z} = \frac{k_z^2}{2m} + \omega_c \left(n + \frac{1}{2} \right). \quad (153)$$

where n is the Landau level index [see Fig. 4 c)]. The spectrum thus takes a quasi one-dimensional form of dispersing Landau levels – a general feature of 3D systems in a magnetic field. We have to keep in mind that the Landau levels are still highly degenerate due to the k_y quantum number (this not being k_x simply reflects an arbitrariness in the gauge choice).

Let us compute the density of states of a system of size L^3

$$\begin{aligned} \frac{dN}{dE}(E) &= \frac{1}{L^3} \sum_n \frac{L^2}{2\pi \ell^2} \sum_{k_z} \delta(E - E_{n,k_z}) \\ &= \frac{1}{2\pi \ell^2} \sum_n \int \frac{dk_z}{2\pi} \delta \left[E - \frac{k_z^2}{2m} - \omega_c \left(n + \frac{1}{2} \right) \right] \\ &= \frac{(2m)^{3/2} \omega_c}{8\pi^2} \sum_n \frac{1}{\sqrt{E - \omega_c(n + 1/2)}}. \end{aligned} \quad (154)$$

Comparing this to the 3D system without magnetic field,

$$\frac{dN}{dE}(E) = \frac{1}{L^3} \sum_{\mathbf{k}} \delta[E - \mathbf{k}^2/(2m)] = (2m)^{3/2} \sqrt{E}/(2\pi^2), \quad (155)$$

we observe that the magnetic field enforces a dramatic redistribution of states in the spectrum [see Fig. 4 c)]. The density of states develops a series of singularities located at the bottom of each dispersing Landau level. This has profound implications for the magnetic field dependence of all quantities that are sensitive to the density of states. If the Fermi level is held fixed and B is increased, the bottom of Landau levels will pass the Fermi level successively, each time providing a singular density of states. This leads to magnetic field dependent oscillations of observables. Such oscillations measured in the magnetization of the system go under the name de-Haas-van-Alphen effect. Oscillations in the conductivity are called Shubnikov-de-Haas effect.

We return to semiclassics to get some analytical insight, neglecting both Berry and electric fields

$$\dot{\mathbf{r}} = \frac{\partial \epsilon_{n,\mathbf{k}}}{\partial \mathbf{k}} \quad \dot{\mathbf{k}} = -e\dot{\mathbf{r}} \times \mathbf{B} \quad \Rightarrow \quad \dot{\mathbf{k}} = -e \frac{\partial \epsilon_{n,\mathbf{k}}}{\partial \mathbf{k}} \times \mathbf{B}. \quad (156)$$

Since $\dot{\mathbf{k}}$ is perpendicular to $\partial_{\mathbf{k}} \epsilon_{n,\mathbf{k}}$, the wave packet will stay on the Fermi surface and encircle a closed path in a plane perpendicular to the applied magnetic field. Semiclassical Bohr-Sommerfeld quantization yields the condition

$$\oint_{\mathcal{C}_n} \mathbf{p} \cdot d\mathbf{r} = 2\pi(n + \gamma), \quad (157)$$

on allowed paths \mathcal{C}_n for the wave function to be single valued. Here γ is an extra phase that could be accumulated along the path (for example due to the here neglected Berry curvature contributions). Replacing the momentum

$$\mathbf{p} = \mathbf{k} - e\mathbf{A} = -e(\mathbf{r} \times \mathbf{B} + \mathbf{A}), \quad (158)$$

we obtain

$$\begin{aligned} \oint_{\mathcal{C}_n} \mathbf{p} \cdot d\mathbf{r} &= -e \oint_{\mathcal{C}_n} \mathbf{A} \cdot d\mathbf{r} + e\mathbf{B} \oint_{\mathcal{C}_n} \mathbf{r} \times d\mathbf{r} \\ &= -e\Phi_n + 2e\Phi_n \\ &= 2\pi(n + \gamma), \end{aligned} \quad (159)$$

where $\Phi_n = B_\perp S_n$ is the magnetic flux through the area S_n in configuration space that is enclosed by the path \mathcal{C}_n . Thus,

$$\Phi_n = (n + \gamma)\Phi_0. \quad (160)$$

The path \mathcal{C}_n also encloses an area A_n in momentum space, which due to

$$d\mathbf{k} = e\mathbf{B} \times d\mathbf{r} \quad \Rightarrow \quad |d\mathbf{k}| = eB_\perp |d\mathbf{r}| \quad (161)$$

is related as $A_n = (eB_\perp)^2 S_n$, where B_\perp is the magnetic field component perpendicular to the path in momentum space [see Fig. 4 d)]. Thus

$$A_n = e^2 B_\perp \Phi_n = 2\pi e B_\perp (n + \gamma) = 4\pi^2 \frac{B_\perp}{\Phi_0} (n + \gamma). \quad (162)$$

Now, we change the mindset and keep the area A fixed, while changing the magnetic field. Let combinations (n, B_n) and $(n + 1, B_{n+1})$ correspond to paths enclosing the same area. Subtracting the two equations

$$\frac{1}{B_n} = \frac{4\pi^2}{A\Phi_0} (n + \gamma), \quad \frac{1}{B_{n+1}} = \frac{4\pi^2}{A\Phi_0} (n + \gamma + 1) \quad (163)$$

yields

$$\frac{1}{B_{n+1}} - \frac{1}{B_n} = \frac{4\pi^2}{A\Phi_0}. \quad (164)$$

This means that the frequency of oscillations as a function of $1/B$ directly yields the area in momentum space of the enclosed path. Since the largest (diverging) density of states results from the bottom of Landau levels passing through the Fermi energy, which appear at the *extremal* areas of the Fermi surface (minima and maxima in diameter perpendicular to the applied field direction), the dominant contribution to the above frequency measures the extremal area of the Fermi surface. Rotating the external field allows for a fairly complete map of the Fermi surface shape, if it is of sufficiently simple form.

I. Phonons

1. Quantizing lattice vibrations

So far, we have considered the electrons as dynamical degrees of freedom that are moving in a rigid background of the ionic lattice potential. However, these ion positions are not necessarily as rigid and their motion can back-react on the electronic properties of the crystal. The study of the dynamics of ionic positions around their equilibrium position (where the displacements are small enough so that the crystalline order is not destroyed) is the physics of phonons, i.e., coherent lattice vibrations.

Classically, and in a long-wavelength limit (comparing the wavelength of displacements with the lattice spacing) we can consider a displacement field of a continuous medium $u(x) = x'(x) - x$, where x is the absolute measure of space while $x'(x)$ is the new position of an infinitesimal part of the medium as a result of the displacement. For simplicity, we are only going to be concerned with the case of a 1D system here and only consider displacements along this 1D directions (which will give rise to so-called *acoustic phonons*). Displacements perpendicular to the direction of propagation, which are not captured by our continuous medium approximation, are called *optical* phonons.

The classical displacement field $u(x, t)$ has both elastic (or potential) and kinetic energy

$$E_{\text{el}} = \frac{\lambda}{2} \int dx [\partial_x u(x, t)]^2, \quad E_{\text{kin}} = \frac{\rho_0}{2} \int dx [\partial_t u(x, t)]^2, \quad (165)$$

where ρ_0 is the mass density of the moving ions (i.e., the mass of an ion times their in-

verse distance). We now want to quantize this theory. To that end, we first expand the displacement field in Fourier modes (such that the displacement is real)

$$u(x, t) = \frac{1}{\sqrt{\Omega}} \sum_k [q_k(t)e^{ikx} + q_k^*(t)e^{-ikx}] \quad (166)$$

and re-express the Lagrangian $\mathcal{L} = E_{\text{kin}} - E_{\text{el}}$ using $q_k(t)$. Taking the derivative with respect to $q_k^*(t)$ yields the equation of motion

$$\partial_t^2 q_k(t) + \omega_k^2 q_k(t) = 0, \quad q_k(t) = q_{k,\pm} e^{\pm i\omega_k t} \quad (167)$$

where $\omega_k = c_s|k|$ is the acoustic phonon dispersion and $c_s = \sqrt{\lambda/\rho_0}$ is the speed of sound. We use the equation of motion to substitute the time derivative in the expression of the kinetic energy to obtain

$$E = E_{\text{el}} + E_{\text{kin}} = \sum_k \rho_0 \omega_k^2 [q_k(t)q_k^*(t) + q_k^*(t)q_k(t)]. \quad (168)$$

To obtain a Hamiltonian description, we deduce the canonically conjugate variables

$$Q_k \equiv \sqrt{\rho_0}(q_k + q_k^*), \quad P_k \equiv \partial_t Q_k = -i\omega_k \sqrt{\rho_0}(q_k - q_k^*) \quad (169)$$

in terms of which

$$E = \frac{1}{2} \sum_k [P_k^2 + \omega_k^2 Q_k^2]. \quad (170)$$

Canonical quantization now amounts to elevating these quantities to (hermitian) operators and imposing the commutation relation

$$[\hat{Q}_k, \hat{P}_{k'}] = i\delta_{k,k'}. \quad (171)$$

The problem is essentially a quantum Harmonic oscillator, and, as we just saw in the Landau level eigenfunctions, it is convenient to rewrite the operators in a pair of bosonic creation and annihilation operators

$$\hat{b}_k = \frac{1}{\sqrt{2\omega_k}} (\omega_k \hat{Q}_k + i\hat{P}_k), \quad \hat{b}_k^\dagger = \frac{1}{\sqrt{2\omega_k}} (\omega_k \hat{Q}_k - i\hat{P}_k) \quad (172)$$

which satisfy

$$[\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{k,k'}, \quad [\hat{b}_k, \hat{b}_{k'}] = 0, \quad [\hat{b}_k^\dagger, \hat{b}_{k'}^\dagger] = 0. \quad (173)$$

We thus obtain that the elementary excitations of the crystal, the *phonons*, are bosons created by \hat{b}_k^\dagger with a dispersion ω_k . They are governed by the Hamiltonian

$$\hat{H} = \sum_k \omega_k \left(\hat{b}_k^\dagger \hat{b}_k + \frac{1}{2} \right). \quad (174)$$

The displacement of ions is now endowed with the uncertainty principle, reflected by the fact that their displacement becomes an operator

$$\hat{u}(x) = \frac{1}{\sqrt{\Omega}} \sum_k \frac{1}{\sqrt{2\rho_0\omega_k}} \left(\hat{b}_k e^{ikx} + \hat{b}_k^\dagger e^{-ikx} \right). \quad (175)$$

2. Peierls instability in 1D

Phonons couple to electrons by the deformation of the ionic background potential. This coupling can have various effects on the electronic structure and on the lattice structure. The electron-phonon coupling renormalizes various quantities such as the speed of sound in the material. Here, we want to exemplify possible implications of electron-phonon coupling by a very dramatic effect that appears preferably in (quasi-)1D systems, the so-called Peierls instability. It consists of a static deformation of the crystal that goes along with a opening of a gap in the electronic spectrum. The lattice distortion costs energy, but the opening of a gap in the electronic spectrum yields energy so that the combination of the two effects can be advantageous. A 1D electronic system with a simple $k^2/(2m)$ dispersion has two Fermi points at $k = \pm k_F$. To open a gap, one needs to couple these two points, i.e., one needs to provide a momentum difference of $Q \equiv 2k_F$ to scatter the electrons. The idea is that this momentum is provided by the static lattice deformation, which thus needs to have the same wave vector.

With our understanding that the phonons are bosons, a static lattice deformation requires a state of the lattice with macroscopic occupation of the phonon state with momentum Q . This is realized by a coherent state

$$|\alpha, Q\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\hat{b}_Q^\dagger)^n}{n!} \alpha^n |0\rangle \quad (176)$$

which has the properties

$$\langle \alpha, Q | \hat{b}_Q^\dagger \hat{b}_Q | \alpha, Q \rangle = |\alpha|^2 \quad (177)$$

and

$$\langle \alpha, Q | \hat{u}(x) | \alpha, Q \rangle = \frac{1}{2L\rho_0\omega_Q} (\alpha e^{iQx} + \alpha^* e^{-iQx}). \quad (178)$$

The state can be thought of as a Bose condensate of momentum Q phonons. We will now determine whether such a lattice deformation can be energetically favorable. Since the mode occupation is macroscopic, it suffices to treat the distortion classically and assume

$$u(x) = u_0 \cos Qx, \quad (179)$$

with an amplitude u_0 that is to be determined.

The Hamiltonian describing phonons, electrons (which we take spinless for simplicity), and their coupling reads in real space

$$\hat{H} = \sum_k \frac{k^2}{2m} \hat{c}_k^\dagger \hat{c}_k + \frac{\lambda}{2} \int dx [\partial_x u(x)]^2 - n_0 \int dx dx' V(x-x') [\partial_x u(x)] \hat{\phi}^\dagger(x') \hat{\phi}(x'), \quad (180)$$

where V is the Coulomb interaction. In momentum space, and particularizing on the single phonon mode at momentum Q , we have

$$\hat{H} = \sum_k \frac{k^2}{2m} \hat{c}_k^\dagger \hat{c}_k + \frac{\Omega\rho_0}{4} \omega_Q^2 u_0^2 + iQ\tilde{V}_Q n_0 u_0 \sum_k (\hat{c}_{k+Q}^\dagger \hat{c}_k - \hat{c}_{k-Q}^\dagger \hat{c}_k), \quad (181)$$

where \tilde{V}_Q is the respective Fourier component of the Coulomb interaction.

We now assume that u_0 is small so that we only consider scattering between the phonon states to first order in u_0 . The electronic part of the spectrum is then approximately determined by the eigenvalues of the matrix

$$\begin{pmatrix} \frac{k^2}{2m} & \Delta \\ \Delta^* & \frac{(k-Q)^2}{2m} \end{pmatrix} \quad (182)$$

where $\Delta \equiv -iQ u_0 n \tilde{V}_Q$. They are given by

$$\epsilon_k^\pm = \frac{(k-Q)^2 + k^2}{4m} \pm \sqrt{\left[\frac{(k-Q)^2 - k^2}{4m} \right]^2 + |\Delta|^2}. \quad (183)$$

The total energy of the Fermi sea and the deformed lattice is thus

$$E(u_0) = 2 \sum_{0 \leq k < Q} \epsilon_k^- + \frac{\lambda L Q^2}{4} u_0^2, \quad (184)$$

where the factor of 2 arises from the changing the summation originally ranging from $-Q$ to Q toward only positive k values. To find out whether a finite u_0 is favored, we minimize the energy with respect to u_0

$$\begin{aligned}
0 &= \frac{1}{L} \frac{dE(u_0)}{du_0} \\
&= -16Q^2 mn_0 \tilde{V}_Q^2 u_0 \int_0^Q \frac{dk}{2\pi} \frac{1}{\sqrt{[(k-Q)^2 - k^2]^2 + 16m^2 Q^2 n_0^2 \tilde{V}_Q^2 u_0^2}} + \frac{\lambda}{2} Q^2 u_0 \\
&= (-)^2 16Q^2 mn_0 \tilde{V}_Q^2 u_0 \frac{1}{4\pi Q} \log \left(\frac{-Q^3 + Q\sqrt{Q^4 + 16m^2 Q^2 n_0^2 \tilde{V}_Q^2 u_0^2}}{+Q^3 + Q\sqrt{Q^4 + 16m^2 Q^2 n_0^2 \tilde{V}_Q^2 u_0^2}} \right) + \frac{\lambda}{2} Q^2 u_0 \\
&\approx u_0 \frac{8Q mn_0^2 \tilde{V}_Q^2}{\pi} \log \left(\frac{mn_0 \tilde{V}_Q u_0}{k_F} \right) + \frac{\lambda}{2} Q^2 u_0.
\end{aligned} \tag{185}$$

The solution $u_0 = 0$ is not of interest to us, but

$$\begin{aligned}
u_0 &= \frac{k_F}{mn_0 \tilde{V}_Q} \exp \left[-\frac{k_F \pi \lambda}{8mn_0^2 \tilde{V}_Q^2} \right] \\
&= \frac{2\epsilon_F}{k_F n_0 \tilde{V}_Q} e^{-1/\nu(\epsilon_F)g}
\end{aligned} \tag{186}$$

is. Here, $\nu(\epsilon_F) = 2m/\pi k_F$ is the density of states at the Fermi level and $g = 4n_0^2 \tilde{V}_Q^2/\lambda$ can be interpreted as a coupling constant that describes a phonon-induced electron-electron interaction (hence the power 2 of \tilde{V}_Q). The exponential dependence of the ‘order parameter’ u_0 on the density of states and the coupling constant is a characteristic feature of such weak-coupling instabilities of the Fermi sea, of which we will encounter more examples in the next chapter. As promised, the Peierls instability will open a finite gap in the electronic spectrum for

$$\Delta\epsilon = \epsilon_{k_F}^+ - \epsilon_{k_F}^- = 2|\Delta| = 8\epsilon_F e^{-1/N(\epsilon_F)g}. \tag{187}$$

Thus, the 1D metal has turned into an insulator/semiconductor. As a result of this instability, the charge density of the electrons actually becomes modulated with a wave vector Q . This is called a *charge density wave*. We will discuss density wave instabilities in more detail in the next chapter.

IV. INTERACTIONS IN ITINERANT SYSTEMS

A. Particle-hole excitations

1. In semiconductors

What is a semiconductor? In theory, there is no sharp distinction between the notion of an insulator and a semiconductor: both have a gapped band structure and hence (without electron-electron interactions considered) a gapped zero temperature ground state. The difference is quantitative, namely, the size of the gap in relation to the practically relevant energy scale of thermal activation at room temperature ($300\text{ K} \sim 0.25\text{ meV}$). Materials with multi-eV band gaps (like diamond with $\Delta = 5.5\text{ eV}$) remain insulating at room temperature as thermal activation is exponentially suppressed in $\Delta/(k_B T)$. Semiconductors with gaps of up to 1 eV gain carrier densities of $n \sim 10^3\text{--}10^{11}\text{ cm}^{-3}$ at room temperature, meaning that they are not fully insulating.

A band structure is *gapped* if (at zero temperature) the minimum of the fully unoccupied conduction band is above the maximum of the fully occupied valence band. We speak of a *direct gap* if the minimum of the conduction band and the maximum of the valence band coincide at the same momentum. Otherwise it is an *indirect gap*.

The obvious elementary excitations in semiconductors are electron-hole excitations. To study what interactions do to these excitations, we take

$$\hat{H} = \sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k},\text{v}} \hat{c}_{\text{v},\mathbf{k}}^\dagger \hat{c}_{\text{v},\mathbf{k}} + \epsilon_{\mathbf{k},\text{c}} \hat{c}_{\text{c},\mathbf{k}}^\dagger \hat{c}_{\text{c},\mathbf{k}} \right), \quad (188)$$

as a spinless model of a semiconductor. Here $\hat{c}_{\text{v},\mathbf{k}}^\dagger$ ($\hat{c}_{\text{c},\mathbf{k}}^\dagger$) creates an electron in the valence (conduction) band at momentum \mathbf{k} and we take the dispersions of the two bands, for simplicity, as a $\mathbf{k} \cdot \mathbf{p}$ approximation around a momentum with direct gap Δ

$$\epsilon_{\mathbf{k},\text{v}} = -\frac{\mathbf{k}^2}{2m}, \quad \epsilon_{\mathbf{k},\text{c}} = \frac{\mathbf{k}^2}{2m} + \Delta. \quad (189)$$

In general there is no need for the two effective masses to be equal. The zero temperature (many-body!) ground state is

$$|\Psi_0\rangle = \prod_{\mathbf{k}} c_{\text{v},\mathbf{k}}^\dagger |0\rangle. \quad (190)$$

Particle-hole excitations above it

$$|\mathbf{k}, \mathbf{q}\rangle = c_{\text{c},\mathbf{k}+\mathbf{q}}^\dagger c_{\text{v},\mathbf{k}} |\Psi_0\rangle, \quad (191)$$

carry a possibly nonzero momentum \mathbf{q} and are eigenstates of the Hamiltonian with energy $E_{\mathbf{k},\mathbf{q}} = E_0 + \epsilon_{c,\mathbf{k}+\mathbf{q}} - \epsilon_{v,\mathbf{k}}$ compared to the ground states energy E_0 . For a fixed \mathbf{q} , due to the freedom to choose \mathbf{k} , such electron-hole excitations are possible for a range of energies. The spectrum

$$I(\mathbf{q}, E) = \sum_{\mathbf{k}} \delta[E - (\epsilon_{c,\mathbf{k}+\mathbf{q}} - \epsilon_{v,\mathbf{k}})] \quad (192)$$

forms the so-called *electron-hole continuum* above a \mathbf{q} dependent energy threshold, which for direct gap semiconductors has a minimum at $\mathbf{q} = 0$ where it equals the gap Δ .

We now study how electron-electron interactions can alter the nature of the ground state by favoring a coherent superposition of electron-hole pairs, so-called excitons, energetically. We add the Coulomb interaction term

$$\hat{H}_{\text{int}} = \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha,\beta} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \hat{\phi}_{\beta}^{\dagger}(\mathbf{r}') \hat{\phi}_{\alpha}^{\dagger}(\mathbf{r}) \hat{\phi}_{\alpha}(\mathbf{r}) \hat{\phi}_{\beta}(\mathbf{r}'), \quad (193)$$

where $\alpha, \beta = 1, 2$ are local degrees of freedom (like orbitals or sublattices) that gave rise to the two bands of the semiconductor. Their Fourier transforms are unitarily rotated to the band eigenstates by the Bloch vector $u_{n,\alpha;\mathbf{k}}$ in momentum space

$$\hat{\phi}_{\alpha}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{n=c,v} \sum_{\mathbf{k}} u_{n,\alpha;\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{c}_{n,\mathbf{k}}. \quad (194)$$

We now consider a general trial wave function for an exciton state

$$|\Psi_{\mathbf{q}}\rangle = \sum_{\mathbf{k}} A_{\mathbf{q}}(\mathbf{k}) |\mathbf{k}, \mathbf{q}\rangle, \quad (195)$$

parametrized by the function $A_{\mathbf{q}}(\mathbf{k})$. We can solve the eigenvalue problem $(\hat{H} + \hat{H}_{\text{int}})|\Psi_{\mathbf{q}}\rangle = (E_0 + E_{\mathbf{q}})|\Psi_{\mathbf{q}}\rangle$ in the space of two-particle excitations with momentum \mathbf{q} above the ground state

$$\sum_{\mathbf{k}'} \langle \mathbf{k}, \mathbf{q} | \hat{H} + \hat{H}_{\text{int}} | \mathbf{k}', \mathbf{q} \rangle A_{\mathbf{q}}(\mathbf{k}') = (E_0 + E_{\mathbf{q}}) A_{\mathbf{q}}(\mathbf{k}). \quad (196)$$

The matrix elements are

$$\langle \mathbf{k}, \mathbf{q} | \hat{H} | \mathbf{k}', \mathbf{q} \rangle = \delta_{\mathbf{k},\mathbf{k}'} E_{\mathbf{k},\mathbf{q}} \quad (197)$$

and

$$\begin{aligned} \langle \mathbf{k}, \mathbf{q} | \hat{H}_{\text{int}} | \mathbf{k}', \mathbf{q} \rangle &= \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha,\beta} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \langle \mathbf{k}, \mathbf{q} | \hat{\phi}_{\beta}^{\dagger}(\mathbf{r}') \hat{\phi}_{\alpha}^{\dagger}(\mathbf{r}) \hat{\phi}_{\alpha}(\mathbf{r}) \hat{\phi}_{\beta}(\mathbf{r}') | \mathbf{k}', \mathbf{q} \rangle \\ &= \frac{1}{\Omega^2} \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha,\beta} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \sum_{n, n', m, m'=c,v} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} e^{i(\mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}'} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \\ &\quad \times u_{n',\alpha;\mathbf{k}_2}^* u_{n,\alpha;\mathbf{k}_1} u_{m',\beta;\mathbf{k}_4}^* u_{m,\beta;\mathbf{k}_3} \langle \mathbf{k}, \mathbf{q} | \hat{c}_{m',\mathbf{k}_4}^{\dagger} \hat{c}_{n',\mathbf{k}_2}^{\dagger} \hat{c}_{n,\mathbf{k}_1} \hat{c}_{m,\mathbf{k}_3} | \mathbf{k}', \mathbf{q} \rangle. \end{aligned} \quad (198)$$

Since we are only interested in small momentum transfers (the main contributions come from around $\mathbf{k} \sim \mathbf{0}$), we can approximate

$$\sum_{\alpha} u_{m',\alpha;\mathbf{k}_1}^* u_{m,\alpha;\mathbf{k}_2} \approx \delta_{m,m'} \quad (199)$$

yielding

$$\begin{aligned} \langle \mathbf{k}, \mathbf{q} | \hat{H}_{\text{int}} | \mathbf{k}', \mathbf{q} \rangle &= \frac{1}{\Omega^2} \int d\mathbf{r} d\mathbf{r}' \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \sum_{n, m=c, v} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} e^{i(\mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}'} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \\ &\times \langle \mathbf{k}, \mathbf{q} | \hat{c}_{m, \mathbf{k}_4}^\dagger \hat{c}_{n, \mathbf{k}_2}^\dagger \hat{c}_{n, \mathbf{k}_1} \hat{c}_{m, \mathbf{k}_3} | \mathbf{k}', \mathbf{q} \rangle. \end{aligned} \quad (200)$$

The expectation value of the second quantized operators can, for $\mathbf{k} \neq \mathbf{k}'$ be replaced by

$$\begin{aligned} \langle \mathbf{k}, \mathbf{q} | \hat{c}_{m, \mathbf{k}_4}^\dagger \hat{c}_{n, \mathbf{k}_2}^\dagger \hat{c}_{n, \mathbf{k}_1} \hat{c}_{m, \mathbf{k}_3} | \mathbf{k}', \mathbf{q} \rangle &\rightarrow -\delta_{m,v} \delta_{n,c} \delta_{\mathbf{k}+\mathbf{q}, \mathbf{k}_2} \delta_{\mathbf{k}, \mathbf{k}_3} \delta_{\mathbf{k}', \mathbf{k}_4} \delta_{\mathbf{k}'+\mathbf{q}, \mathbf{k}_1} \\ &- \delta_{n,v} \delta_{m,c} \delta_{\mathbf{k}+\mathbf{q}, \mathbf{k}_4} \delta_{\mathbf{k}, \mathbf{k}_1} \delta_{\mathbf{k}', \mathbf{k}_2} \delta_{\mathbf{k}'+\mathbf{q}, \mathbf{k}_3} \end{aligned} \quad (201)$$

resulting in

$$\begin{aligned} \langle \mathbf{k}, \mathbf{q} | \hat{H}_{\text{int}} | \mathbf{k}', \mathbf{q} \rangle &= -\frac{2}{\Omega^2} \int d\mathbf{r} d\mathbf{r}' e^{i(\mathbf{k}' - \mathbf{k}) \cdot (\mathbf{r} - \mathbf{r}')} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \\ &= -\frac{2}{\Omega} \frac{2\pi e^2}{(\mathbf{k} - \mathbf{k}')^2}. \end{aligned} \quad (202)$$

We now include the electrostatic environment of the medium phenomenologically by introducing the dielectric constant, replacing $e^2 \rightarrow e^2/\epsilon$ in the interaction strength. The eigenvalue equation for $A_{\mathbf{q}}(\mathbf{k})$ now reads

$$(E_{\mathbf{q}, \mathbf{k}} - E) A_{\mathbf{q}}(\mathbf{k}) - \frac{1}{\Omega} \sum_{\mathbf{k}'} \frac{4\pi e^2}{\epsilon(\mathbf{k} - \mathbf{k}')^2} A_{\mathbf{q}}(\mathbf{k}') = 0. \quad (203)$$

Returning to real space

$$\tilde{A}_{\mathbf{q}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} A_{\mathbf{q}}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (204)$$

and using the dispersions Eq. (189) we obtain (shifting \mathbf{k} to $\mathbf{k} - \mathbf{q}/2$)

$$\left[-\frac{\nabla^2}{2(m/2)} - \frac{e^2}{\epsilon|\mathbf{r}|} \right] \tilde{A}_{\mathbf{q}}(\mathbf{r}) = \left[E - E_0 - \Delta - \frac{\mathbf{q}^2}{2(2m)} \right] \tilde{A}_{\mathbf{q}}(\mathbf{r}), \quad (205)$$

which is exactly the Schroedinger equation for the hydrogen atom with reduced mass $\mu_{\text{ex}} = m_1 m_2 / (m_1 + m_2) = m/2$ and total mass $M_{\text{ex}} = 2m$. The spectrum is given by

$$E_{\mathbf{q}} = E_0 + \Delta - \frac{\mu_{\text{ex}} e^4}{2\epsilon^2 n^2} + \frac{\mathbf{q}^2}{2M_{\text{ex}}}, \quad (206)$$

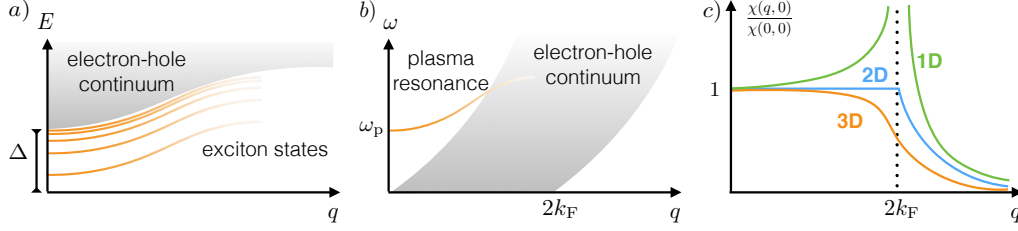


Figure 5. a) Excitation spectrum of a direct gap semiconductor with a gap Δ and interaction-induced exciton bound states in the gap. b) Excitation spectrum of a 3D metal as deduced from the charge susceptibility with electron-hole continuum and the interaction-induced plasma resonance. c) Form of the singularity of the static ($\omega = 0$) charge susceptibility of metals in different dimensions.

which implies the existence of bound states below the electron-hole continuum. [See Fig. 5 a)] The fact that these excitations have a sharp dispersion relation $E_{\mathbf{q}}$ qualifies them to be called a *quasiparticle* in condensed matter. This quasiparticle is called *exciton*. Quasiparticles are a very powerful concept covering many interaction effects in many-body systems. A quasiparticle can only exist because of the many-electron background. In the case at hand, they are a collective excitation that includes the polarization from all electrons. Excitons carry no charge and are bosonic in character, as they are made of two fermions. Bose-Einstein condensation of excitons has been observed experimentally.

2. In metals

a. RPA susceptibility As in semiconductors, the elementary excitations in metals are particle-hole excitations. However, in metals they can appear at arbitrarily small energies. As a result, the effective Coulomb interaction is not only rescaled as is the case in semiconductors due to the dipolar electric environment, but substantially modified taking the form $e^{-r/l}/r$, as we will derive below.

We recall that the noninteracting linear response of a metal to potential perturbation is given by

$$\delta\rho(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega)V(\mathbf{q}, \omega), \quad (207)$$

with

$$\chi_0(\mathbf{q}, \omega) = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega - i\eta}, \quad (208)$$

where $n_{\mathbf{k}} = 1/(e^{\beta\epsilon_{\mathbf{k}}} + 1)$ is the occupation number of the band according to the Fermi-Dirac distribution. We now want to see how the Coulomb interaction changes this response. The redistribution of electron density $\delta\rho(\mathbf{q}, \omega)$ due to the external potential $V(\mathbf{q}, \omega)$ sources an additional Coulomb potential if interactions are considered. The latter is determined by the Poisson equation

$$\nabla^2 V_C(\mathbf{r}, t) = -4\pi e^2 \delta\rho(\mathbf{r}, t), \quad V_C(\mathbf{q}, \omega) = \frac{4\pi e^2}{\mathbf{q}^2} \delta\rho(\mathbf{q}, \omega). \quad (209)$$

The total potential felt by the electrons is thus the sum of the two contributions

$$\begin{aligned} V_{\text{tot}}(\mathbf{q}, \omega) &= V(\mathbf{q}, \omega) + V_C(\mathbf{q}, \omega) \\ &= V(\mathbf{q}, \omega) + \frac{4\pi e^2}{\mathbf{q}^2} \delta\rho(\mathbf{q}, \omega), \end{aligned} \quad (210)$$

which is a self-consistent equation for $\delta\rho(\mathbf{q}, \omega)$ when considered together with

$$\delta\rho(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega) V_{\text{tot}}(\mathbf{q}, \omega). \quad (211)$$

Solving for $V_{\text{tot}}(\mathbf{q}, \omega)$, we can write

$$V_{\text{tot}}(\mathbf{q}, \omega) = \frac{1}{\epsilon(\mathbf{q}, \omega)} V(\mathbf{q}, \omega), \quad (212)$$

where

$$\epsilon(\mathbf{q}, \omega) = 1 - \frac{4\pi e^2}{\mathbf{q}^2} \chi_0(\mathbf{q}, \omega) \quad (213)$$

is called the *dynamical dielectric function* that describes the renormalization of the external potential due to the electrons in the metal.

Inserting this in the equation for $\delta\rho(\mathbf{q}, \omega)$, we find

$$\delta\rho(\mathbf{q}, \omega) = \chi(\mathbf{q}, \omega) V(\mathbf{q}, \omega), \quad (214)$$

where response functions including interaction effects is given by

$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{\epsilon(\mathbf{q}, \omega)} = \frac{\chi_0(\mathbf{q}, \omega)}{1 - \frac{4\pi e^2}{\mathbf{q}^2} \chi_0(\mathbf{q}, \omega)}, \quad (215)$$

which is called the *random phase approximation* (RPA) form of the response function. (The name stems from the fact that, when $\chi(\mathbf{q}, \omega)$ is computed from a perturbative expansion

in the interaction strength, certain terms are exactly summed in the above form to infinite order, while others which are assumed to cancel on average due to random relative phases are not summed.)

Both $\chi_0(\mathbf{q}, \omega)$ and $\chi(\mathbf{q}, \omega)$ are complex valued quantities. The real and imaginary parts contain distinct information about the physics of the system. Divergences in the real part signal instabilities of the ground state toward symmetry-breaking states. $\chi(\mathbf{q}, \omega)$ can diverge if the interaction is sufficiently strong such that the denominator goes to zero (evidencing that interactions are necessary for such an instability). We will defer the study of instabilities for later. The imaginary part contains information about excitations of the metal which will be our primary interest for now.

First, for the noninteracting case of $\chi_0(\mathbf{q}, \omega)$, we can use

$$\lim_{\eta \rightarrow 0^+} \frac{1}{x - i\eta} = \mathcal{P}(x^{-1}) + i\pi\delta(x), \quad (216)$$

where \mathcal{P} denotes the Cauchy principal value to obtain

$$\begin{aligned} \text{Re } \chi_0(\mathbf{q}, \omega) &= \frac{1}{\Omega} \sum_{\mathbf{k}} \mathcal{P} \left(\frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega} \right) \\ \text{Im } \chi_0(\mathbf{q}, \omega) &= \frac{\pi}{\Omega} \sum_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega). \end{aligned} \quad (217)$$

The imaginary part is exactly what Fermi's golden rule would yield for the transition rate from the ground state to an excited state with an electron-hole pair excitation. In a 3D metal with spherical Fermi surface, excitations with arbitrarily small energies are possible in a range of momenta $|\mathbf{q}| \leq 2k_F$, where k_F is the Fermi wave vector. For small momentum transfer and finite frequencies ω , there are no excitations in the particle hole continuum.

We will now explore a collective excitation induced by the Coulomb interaction. This so-called *plasma resonance* appears at small momenta and finite frequency, where no continuum of particle-hole excitations is allowed. To study it, we consider the RPA susceptibility and expand all quantities entering it in small momenta $|\mathbf{q}| \ll k_F$

$$\begin{aligned} \epsilon_{\mathbf{k}+\mathbf{q}} &= \epsilon_{\mathbf{k}} + \mathbf{q} \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} + \cdots \\ n_{\mathbf{k}+\mathbf{q}} &= n_{\mathbf{k}} + \frac{\partial n}{\partial \epsilon} \mathbf{q} \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}. \end{aligned} \quad (218)$$

At zero temperature, $\partial_{\epsilon} n = -\delta(\epsilon)$ (keep in mind that all energies are measured with respect to the Fermi energy, or the chemical potential) and we can write $\mathbf{q} \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} = v_F q \cos \theta$, where

θ is the angle between the (fixed) vector \mathbf{q} and \mathbf{k} . The bare susceptibility becomes

$$\begin{aligned}
\chi_0(\mathbf{q}, \omega) &= - \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{v_F q \cos \theta \delta(\epsilon_{\mathbf{k}})}{v_F q \cos \theta - \omega - i\eta} \\
&= - \frac{(2\pi)}{(2\pi)^3} \int_0^\pi d\theta \frac{k_F^2}{v_F} \sin \theta \frac{v_F q \cos \theta}{v_F q \cos \theta - \omega - i\eta} \\
&= - \frac{k_F^2}{(2\pi)^2 v_F} \int_{-1}^1 d\xi \frac{\xi}{\xi - \frac{\omega + i\eta}{v_F q}} \\
&= \frac{k_F^2}{(2\pi)^2 v_F} \frac{2}{3} \left(\frac{v_F q}{\omega + i\eta} \right)^2 \left[1 + \frac{3}{5} \left(\frac{v_F q}{\omega + i\eta} \right)^2 \right] + \mathcal{O}(q^4) \\
&= \frac{n_{k_F} q^2}{2m(\omega + i\eta)^2} \left[1 + \frac{3}{5} \left(\frac{v_F q}{\omega + i\eta} \right)^2 \right] + \mathcal{O}(q^4).
\end{aligned} \tag{219}$$

We used the integral

$$\int_{-1}^1 d\xi \frac{\xi}{\xi - 1/b} = 2 - \frac{2}{b} \arctan(b) = -\frac{2}{3} b^2 \left[1 + \frac{3}{5} b^2 \right] + \mathcal{O}(b^6). \tag{220}$$

We first need the q^2 term to find that, following Eq. (213), the dielectric function has a characteristic frequency dependence

$$\lim_{q \rightarrow 0} \epsilon(\mathbf{q}, \omega) = 1 - \frac{\omega_p^2}{\omega^2} \tag{221}$$

where the so-called plasma frequency is given by $\omega_p^2 = 4\pi e^2 n_{k_F}/m$.

Second, we use Eq. (219) to rewrite the RPA susceptibility as

$$\begin{aligned}
\chi(\mathbf{q}, \omega) &\approx \frac{n_{k_F} q^2 R(q, \omega)^2}{2m(\omega + i\eta)^2 - 8\pi e^2 n_{k_F} R(q, \omega)^2} \\
&= \frac{n_{k_F} q^2 R(q, \omega)}{4m\omega_p} \left(\frac{1}{\omega + i\eta - \omega_p R(q, \omega)} - \frac{1}{\omega + i\eta + \omega_p R(q, \omega)} \right)
\end{aligned} \tag{222}$$

with

$$R(q, \omega)^2 = 1 + \frac{3v_F^2 q^2}{5\omega^2}. \tag{223}$$

Now, we can use Eq. (216) to compute

$$\text{Im } \chi(\mathbf{q}, \omega) = \frac{\pi n_{k_F} q^2 R(q, \omega)}{2m\omega_p} [\delta(\omega - \omega_p R(q, \omega_p)) - \delta(\omega + \omega_p R(q, \omega_p))]. \tag{224}$$

This has an excitation with well-defined dispersion relation

$$\omega(\mathbf{q}) = \omega_p R(q, \omega_p) \approx \omega_p \left(1 + \frac{3v_F^2}{10\omega_p^2} q^2 \right), \tag{225}$$

i.e., a quasiparticle. It is called *plasma resonance* and the associated *plasmon* is again bosonic in character. The plasma resonance coexists with the electron-hole continuum at larger q , but is damped due to the decay into electron-hole excitations. [See Fig. 5 b)] Actual values for the plasma frequency are typically in the range of a few eV. The plasma resonance can be understood from classical electrodynamics. If the mobile electrons are shifted with respect to the ions by a rigid displacement \mathbf{r} , there results a polarization-induced electric field $\mathbf{E} = 4\pi e n_{k_F} \mathbf{r}$. This exerts a force on the electron cloud and the equation of motion becomes that of a harmonic oscillator

$$m\ddot{\mathbf{r}} = -e\mathbf{E} = -4\pi e^2 n_{k_F} \mathbf{r}. \quad (226)$$

The eigenfrequency of that oscillator is precisely the plasma frequency

$$\omega_p^2 = \frac{4\pi e^2 n_{k_F}}{m}. \quad (227)$$

b. Thomas-Fermi screening In closing this section, we return to our initial question, namely the form of the effective interaction potential, once the screening by the mobile electrons in the metal is taken into account. This is most easily found by taking the $\omega \rightarrow 0$ limit, i.e., the static limit, of the self-consistent potential using the dielectric function. We start from the first line of Eq. (219) (we multiply the susceptibility by 2 here to account for the spin degree of freedom and connect to known results below)

$$\chi_0(\mathbf{q}, 0) = -\frac{4\pi}{(2\pi)^3} \frac{k_F^2}{v_F} = -\frac{3n_{k_F}}{2\epsilon_F} \quad (228)$$

and, following Eq. (213) we find the static dielectric function

$$\epsilon(\mathbf{q}, 0) = 1 + \frac{k_{TF}^2}{q^2}, \quad (229)$$

written in terms of the *Thomas-Fermi* wave vector $k_{TF}^2 = 6\pi e^2 n_{k_F} / \epsilon_F$ which quantifies the screening by the mobile electrons. To see how the profile of the Coulomb interaction is modified by this screening, consider the potential of a bare charge $V(\mathbf{q}) = 4\pi e^2 / q^2$ and how it modifies the total potential

$$V_{\text{tot}}(\mathbf{q}) = \frac{4\pi e^2}{q^2 + k_{TF}^2}. \quad (230)$$

We observe that k_{TF}^2 is a cutoff of the potential for small q , i.e., long distances. This becomes even clearer in the Fourier transformed version

$$V_{\text{tot}}(\mathbf{r}) = \frac{e^2}{r^2} e^{-k_{TF} r}, \quad (231)$$

showing the exponential screening of the Coulomb potential at long distances. In a metal, the screening length is comparable to the Fermi momentum. The Thomas-Fermi screening implies that electric fields cannot penetrate a metal on distances larger than k_{TF}^{-1} , i.e., a few interatomic distances.

c. Singularities in lower dimensions The bare static susceptibility can be computed exactly in different dimensions for a fully isotropic Fermi surface and a quadratic dispersion. The results are

$$\begin{aligned}\chi_0^{(1\text{D})}(q, 0) &= -\frac{1}{2\pi q} \log \left| \frac{s+2}{s-2} \right|, \\ \chi_0^{(2\text{D})}(q, 0) &= -\frac{1}{2\pi} \left[1 - \sqrt{1 - 4/s^2} \Theta(s-2) \right], \\ \chi_0^{(3\text{D})}(q, 0) &= -\frac{k_{\text{F}}}{2\pi^2} \left[1 - \frac{s}{4} \left(1 - \frac{4}{s^2} \right) \log \left| \frac{s+2}{s-2} \right| \right],\end{aligned}\tag{232}$$

with $s = q/k_{\text{F}}$. At $s = 2$, i.e., for scattering processes across the Fermi surface, χ_0 is not smooth. [See Fig. 5 c)] However, the order of non-smoothness depends on the dimension and is more severe for smaller dimensions. In particular, in 1D the susceptibility is diverging at $q = 2k_{\text{F}}$ signaling an instability of the electronic system.

B. Fermi liquid theory

What happens to a noninteracting fermi sea ground state of a metal when interactions are added? This is a highly nontrivial question and a multitude of instabilities are conceivable, including symmetry breaking states (magnetism, superconductivity, density waves), Mott insulators and others. The main message of this section, and the core statement of Fermi liquid theory is: In many cases not all that much happens. The character and key properties of the Fermi sea survive the presence of interactions with some conceptual modifications. This bold statement is valid in 3D for weak repulsive interactions. It is a blessing for us, since we rely very much on the conducting properties of metals. If they were unstable, it would pose a technological challenge.

1. Quasiparticles

At the basis of the Fermi liquid theory are so-called quasiparticles. They are a sharply defined concept for excitations above and very close to the Fermi sea. To get some intuition

about this, we consider a system with a filled Fermi sea, dispersion $\epsilon_{\mathbf{k}} = \mathbf{k}^2/(2m)$, and Fermi momentum k_F . We consider a state with this Fermi sea filled and one additional electron at some \mathbf{k} with $|\mathbf{k}| > k_F$. This state is an eigenstate of the noninteracting Hamiltonian, but if electron-electron interactions

$$\hat{H}_{\text{int}} = \int d\mathbf{r} d\mathbf{r}' \sum_{\alpha, \beta} V(\mathbf{r} - \mathbf{r}') \phi_{\beta}^{\dagger}(\mathbf{r}') \phi_{\alpha}^{\dagger}(\mathbf{r}) \phi_{\alpha}(\mathbf{r}) \phi_{\beta}(\mathbf{r}'), \quad (233)$$

are considered it will have a nonvanishing decay amplitude into other states. Specifically, we consider the screened Coulomb interactions

$$V(\mathbf{q}) = \frac{4\pi e^2}{q^2 + k_{\text{TF}}^2}. \quad (234)$$

The lowest order effect of the interaction that couples to the electron at \mathbf{k} is to create an extra particle-hole pair with momenta $(\mathbf{k}' + \mathbf{q})$ and \mathbf{k}' and at the same time to shift the momentum of the extra electron to $(\mathbf{k} - \mathbf{q})$. [See Fig. 6 a)] Momentum is conserved in this process because

$$\mathbf{k} = (\mathbf{k} - \mathbf{q}) - \mathbf{k}' + (\mathbf{k}' + \mathbf{q}) \quad (235)$$

and energy conservation requires

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}'} + \epsilon_{\mathbf{k}'+\mathbf{q}}. \quad (236)$$

(We will use a convention in which $\epsilon_{\mathbf{k}}$ is measured relative to the Fermi energy, i.e., it includes the chemical potential and is zero near the Fermi surface.)

We now want to calculate the total decay rate of the initial state by summing over all possible final states (i.e., all \mathbf{q} and \mathbf{k}'). Fermi's golden rule yields

$$\frac{1}{\tau_{\mathbf{k}}} = 2 \frac{2\pi}{\Omega^2} \sum_{\mathbf{k}', \mathbf{q}} |V(\mathbf{q})|^2 n_{\mathbf{k}'} (1 - n_{\mathbf{k}-\mathbf{q}}) (1 - n_{\mathbf{k}'+\mathbf{q}}) \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}'+\mathbf{q}}), \quad (237)$$

where the factor of 2 is for the spin degeneracy. The factors $n_{\mathbf{k}'}(1 - n_{\mathbf{k}-\mathbf{q}})(1 - n_{\mathbf{k}'+\mathbf{q}})$ ensure that the final state is indeed available by the Pauli principle. After some algebra, that we relegate to an exercise, we obtain the following approximation for the lifetime of the excitation

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{N(\epsilon_F)}{8\pi v_F^2} \epsilon_{\mathbf{k}}^2 \int d\mathbf{q} |V(\mathbf{q})|^2, \quad (238)$$

where $N(\epsilon_F) = m^* k_F / \pi^2$ is the density of states at the Fermi level.

Exercise: Fill in the missing steps to compute the quasiparticle life time.

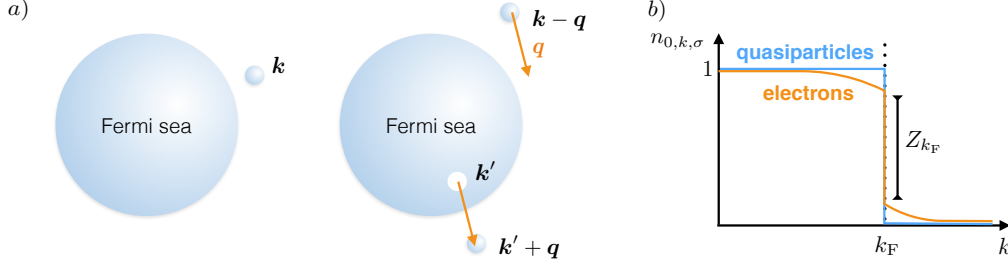


Figure 6. a) Dominant decay processes for a single particle excitation above the filled Fermi sea. b) Momentum distribution function at zero temperature in an interacting Fermi liquid for the original electrons (orange) and the quasiparticles (blue). The latter follow the Fermi-Dirac distribution, while the former have a smaller step-like singularity that equates to the quasiparticle weight Z_{k_F} .

The key feature of this result is that $\tau_{\mathbf{k}} \propto \epsilon_{\mathbf{k}}^{-2}$, i.e., the lifetime becomes infinitely long close to the Fermi surface, while excitations at higher energy decay much faster. This is indicative of a well-defined quasiparticle concept at energies close to the Fermi level. It comes about because of the reduced phase space available for scattering processes that obey momentum conservation, energy conservation, and the Pauli principle simultaneously for small excitation energies.

2. Basics of Landau Fermi liquids

Landau's theory of Fermi liquid can be motivated from microscopic considerations, but for efficiency, we present it as an axiomatic effective theory here. The basic axiom is that there is a *one-to-one* mapping between the excitations above the noninteracting Fermi sea (free electrons) and the excitations above the interacting many-body ground states (quasiparticles). We denote the momentum distribution function of the quasiparticles by $n_{\mathbf{k},\sigma}$ and that of the electrons by $\tilde{n}_{\mathbf{k},\sigma}$, where $\sigma = \pm$ denotes the spin. The total number of electrons equals the number of quasiparticles

$$N = \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \tilde{n}_{\mathbf{k},\sigma}. \quad (239)$$

One now postulates that the distribution function of the *quasiparticles* in equilibrium follows the Fermi-Dirac distribution $n_{0,\mathbf{k},\sigma}$. As a consequence, the *electronic* distribution function

becomes distorted. In particular, the jump at k_F at $T = 0$ is reduced from 1 to a smaller value (but there is still a jump). The jump height is called quasi-particle weight Z_{k_F} . [See Fig. 6 b)]

The object of interest in the Fermi liquid theory are the deviations from the equilibrium quasiparticle distribution function

$$\delta n_{\mathbf{k},\sigma} = n_{\mathbf{k},\sigma} - n_{0,\mathbf{k},\sigma}, \quad (240)$$

which is a small expansion parameter in the theory. Central is an expansion of the energy as a functional of this parameter

$$E[\delta n] = E_0 + \sum_{\mathbf{k},\sigma} \epsilon_{\sigma,\mathbf{k}} \delta n_{\mathbf{k},\sigma} + \frac{1}{\Omega} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma,\sigma'} f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \delta n_{\mathbf{k},\sigma} \delta n_{\mathbf{k}',\sigma'} + \mathcal{O}(\delta n^3), \quad (241)$$

where E_0 is the ground state energy, and $\epsilon_{\sigma,\mathbf{k}}$ as well as $f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'}$ are phenomenological parameters at this stage which can be determined from a microscopic derivation or experimental input. The variational derivative with respect to δn yields a renormalized effective dispersion of the quasiparticles due to the interaction with the perturbed background quasiparticles

$$\tilde{\epsilon}_{\mathbf{k},\sigma} = \epsilon_{\mathbf{k},\sigma} + \frac{1}{\Omega} \sum_{\mathbf{k}',\sigma'} f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \delta n_{\mathbf{k}',\sigma'}. \quad (242)$$

To obtain a more practical set of parameters in a perturbative regime, one ignores the radial dependence of $f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'}$ on \mathbf{k} and \mathbf{k}' so that the only relevant variable is the angle θ between \mathbf{k} and \mathbf{k}' , which are both assumed to lie on the Fermi surface. We can then expand $f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'}$ in Legendre polynomials

$$f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \approx f_{\theta;\sigma,\sigma'} = \sum_{l=0}^{\infty} (f_l^s + \sigma\sigma' f_l^a) P_l(\cos \theta), \quad (243)$$

where we have also split up each coefficient into a spin-symmetric f_l^s and a spin-asymmetric part f_l^a . When rescaled by the density of states at the Fermi level $\nu(\epsilon_F)$, these parameters are known as the *Landau parameters* of the theory

$$F_l^s = \nu(\epsilon_F) f_l^s, \quad F_l^a = \nu(\epsilon_F) f_l^a. \quad (244)$$

3. Compressibility and susceptibility

As an application of the Fermi liquid theory, we compute its compressibility and magnetic susceptibility. The former is defined by

$$\kappa = -\frac{1}{\Omega} \left(\frac{\partial \Omega}{\partial p} \right)_{T,N}, \quad (245)$$

where p is the uniform pressure exerted on the system. The quasiparticle energy levels are affected by the pressure as

$$\begin{aligned} d\epsilon_{\mathbf{k},\sigma} &= \frac{\partial \epsilon_{\mathbf{k},\sigma}}{\partial p} dp \\ &= \frac{\partial \epsilon_{\mathbf{k},\sigma}}{\partial \mathbf{k}} \cdot \frac{\partial \mathbf{k}}{\partial \Omega} \frac{\partial \Omega}{\partial p} dp \\ &= \mathbf{v}_{\mathbf{k}} \cdot \frac{\mathbf{k}}{3} \kappa^{(0)} dp \\ &\approx \frac{2\epsilon_F}{3} \kappa^{(0)} dp, \end{aligned} \quad (246)$$

where we assumed to be close to the Fermi surface to obtain the last line. We are after the analogous equation for the renormalized quasiparticle dispersion and the compressibility of the Fermi liquid κ

$$d\tilde{\epsilon}_{\mathbf{k},\sigma} = \frac{2\epsilon_F}{3} \kappa dp. \quad (247)$$

To obtain it, we start with the definition of $\tilde{\epsilon}_{\mathbf{k},\sigma}$ and use Eq. (246) for the first term

$$\begin{aligned} d\tilde{\epsilon}_{\mathbf{k},\sigma} &= \frac{2\epsilon_F}{3} \kappa^{(0)} dp + \frac{1}{\Omega} \sum_{\mathbf{k}',\sigma'} f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \frac{\partial \delta n_{\mathbf{k}',\sigma'}}{\partial p} dp \\ &= \frac{2\epsilon_F}{3} \kappa^{(0)} dp + \frac{1}{\Omega} \sum_{\mathbf{k}',\sigma'} f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \frac{\partial \delta n_{\mathbf{k}',\sigma'}}{\partial \tilde{\epsilon}_{\mathbf{k}',\sigma'}} d\tilde{\epsilon}_{\mathbf{k}',\sigma'} \\ &= \frac{2\epsilon_F}{3} \kappa^{(0)} dp - \frac{1}{\Omega} \sum_{\mathbf{k}',\sigma'} f_{\mathbf{k},\mathbf{k}';\sigma,\sigma'} \delta(\tilde{\epsilon}_{\mathbf{k}',\sigma'} - \epsilon_F) \frac{2\epsilon_F}{3} \kappa dp. \end{aligned} \quad (248)$$

Since $\tilde{\epsilon}_{\mathbf{k}',\sigma'}$ is isotropic, this brings about exactly the $l = 0$ Landau parameter and we have

$$\kappa = \kappa^{(0)} - \kappa F_0^s, \quad \kappa = \frac{\kappa^{(0)}}{1 + F_0^s}. \quad (249)$$

Without derivation we also state the unperturbed compressibility of the Fermi liquid $1/\kappa^{(0)} = 2n\epsilon_F/3$.

By similar considerations, we can compute the magnetic susceptibility of the Fermi liquid

$$\begin{aligned} \chi &= \frac{1}{\Omega} \frac{\partial M}{\partial B} \\ &= \frac{\mu_B^2 \nu(\epsilon_F)}{1 + F_0^a}. \end{aligned} \quad (250)$$

Common to Eqs. (249) and (250) is that the Fermi liquid parameter appears in the denominator, indicating the possibility of a divergence (when it reaches the value -1), i.e., an instability of the system. However, for small $F_0^{a/s}$, i.e., weak interactions, the Fermi liquid is stable, as promised. This proof can be extended to all angular momentum channels where a similar form is found. A divergence of the magnetic susceptibility indicates a tendency to (ferro-)magnetic order. This constitutes the so-called Stoner instability which we will encounter again from a more microscopic viewpoint.

C. Transport in metals

In principle, transport is not a concept that requires electron-electron interactions. We still place this section in the chapter on interacting electron systems, as it naturally builds up on the principles of Fermi liquid theory (which is intrinsically interacting), and the results on particle-hole excitations in metals. What follows is often applicable to an interacting Fermi liquid as much as to a system of noninteracting electrons.

1. Linear response and complex analysis

When studying the charge transport properties of a material, the natural object of interest is the conductivity which in linear response is defined by the equation

$$j_\alpha(\mathbf{q}, \omega) = \sum_\beta \sigma_{\alpha,\beta}(\mathbf{q}, \omega) E_\beta(\mathbf{q}, \omega), \quad \alpha, \beta \in \{x, y, z\} \quad (251)$$

Here, we introduced $\sigma_{\alpha,\beta}(\mathbf{q}, \omega)$ in all generality as a tensorial quantity. However, in the following discussion we specialize for simplicity on isotropic systems where $\sigma_{\alpha,\beta}$ is diagonal with equal diagonal elements $\sigma(\mathbf{q}, \omega)$.

We can relate $\sigma(\mathbf{q}, \omega)$ to the susceptibility in the following. For this, we note that current $\mathbf{j}(\mathbf{q}, \omega)$ and charge density $\rho(\mathbf{q}, \omega)$ satisfy the continuity equation

$$\dot{\rho}(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0, \quad (252)$$

which in reciprocal space reads

$$\omega \rho(\mathbf{q}, \omega) - \mathbf{q} \cdot \mathbf{j}(\mathbf{q}, \omega) = 0. \quad (253)$$

Inserting this into Eq. (211) (note that we divide ρ by $(-e)$ to relate it to the number density that was used as $\delta\rho$ in Eq. (211))

$$\begin{aligned}
\chi_0(\mathbf{q}, \omega) &= -\frac{\rho(\mathbf{q}, \omega)}{eV(\mathbf{q}, \omega)} \\
&= -\frac{\mathbf{q} \cdot \mathbf{j}(\mathbf{q}, \omega)}{e\omega V(\mathbf{q}, \omega)} \\
&= -\frac{\sigma(\mathbf{q}, \omega) \mathbf{q} \cdot \mathbf{E}(\mathbf{q}, \omega)}{e\omega V(\mathbf{q}, \omega)} \\
&= -\frac{\sigma(\mathbf{q}, \omega)}{\omega} \frac{i\mathbf{q}^2 V(\mathbf{q}, \omega)}{eV(\mathbf{q}, \omega)},
\end{aligned} \tag{254}$$

where we used the first Maxwell equation $e\mathbf{E}(\mathbf{q}, \omega) = -i\mathbf{q}V(\mathbf{q}, \omega)$. In summary

$$\chi_0(\mathbf{q}, \omega) = -i\frac{\mathbf{q}^2}{e^2\omega}\sigma(\mathbf{q}, \omega), \quad \epsilon(\mathbf{q}, \omega) = 1 + i\frac{4\pi}{\omega}\sigma(\mathbf{q}, \omega). \tag{255}$$

From our discussion of the plasma resonance, we had deduced that for small $q \ll k_F$ the dielectric function takes the form $\epsilon(0, \omega) = 1 - \omega_p^2/\omega^2$, which implies for the conductivity in this limit

$$\sigma(\omega) = i\frac{\omega_p^2}{4\pi\omega}. \tag{256}$$

Is the conductivity purely imaginary in the limit of small frequency and momenta? This is not the case, as we can directly see from computing the Kramers-Kronig relation between imaginary and real part

$$\begin{aligned}
\text{Re } \sigma(\omega) &= -\frac{1}{\pi} \mathcal{P} \left[\int_{-\infty}^{\infty} d\omega' \frac{\text{Im } \sigma(\omega')}{\omega - \omega'} \right] \\
\text{Im } \sigma(\omega) &= +\frac{1}{\pi} \mathcal{P} \left[\int_{-\infty}^{\infty} d\omega' \frac{\text{Re } \sigma(\omega')}{\omega - \omega'} \right].
\end{aligned} \tag{257}$$

Using the form of Eq. (256), we obtain for any finite ω that $\text{Re } \sigma(\omega) = 0$ simply by shifting the integration variable ω' by $\omega/2$. For $\omega = 0$ we obtain a divergence which using the Cauchy principal value yields

$$\text{Re } \sigma(\omega) = \frac{\omega_p^2}{4} \delta(\omega), \quad \text{Im } \sigma(\omega) = \frac{\omega_p^2}{4\pi\omega}. \tag{258}$$

This tells us that the metal is perfectly conducting (finite conductivity comes results from disorder scattering, which will be considered below). Furthermore, the conductivity obeys the so-called *f sum rule* following from complex analysis

$$\int_0^{\infty} d\omega' \text{Re } \sigma(\omega') = \frac{1}{2} \int_{-\infty}^{\infty} d\omega' \text{Re } \sigma(\omega') = \frac{\omega_p^2}{8} = \frac{\pi e^2 n}{2m}, \tag{259}$$

where n is the carrier density.

2. Boltzmann transport theory

To include the effect of impurity scattering, we utilize Boltzmann's transport theory, which is an efficient semiclassical tool to compute transport responses. The central object of interest is the distribution function

$$f(\mathbf{k}, \mathbf{r}, t) \quad (260)$$

in phase space which gives the number of (quasi-)particles residing in a phase space volume $d^3\mathbf{r}d^3\mathbf{k}/(2\pi)^3$ at a point (\mathbf{k}, \mathbf{r}) and at time t . For this semiclassical picture of phase space to be applicable, we restrict ourselves to phenomena at small wave numbers and small energies

$$q \ll k_F, \quad \omega \ll \epsilon_F. \quad (261)$$

From this definition there follows the total number of particles as

$$N = 2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} d^3\mathbf{r} f(\mathbf{k}, \mathbf{r}, t) \quad (262)$$

and the equilibrium distribution function (i.e., in absence of perturbations to the system) as the Fermi-Dirac distribution

$$f_0(\mathbf{k}, \mathbf{r}, t) = \frac{1}{e^{\beta \epsilon_{\mathbf{k}}} + 1}. \quad (263)$$

The key equation obeyed by $f(\mathbf{k}, \mathbf{r}, t)$ is the Boltzmann equation which says that the total time derivative of $f(\mathbf{k}, \mathbf{r}, t)$ equals a functional called the *collision integral* which incorporates the scattering processes

$$\frac{d}{dt} f(\mathbf{k}, \mathbf{r}, t) = \left(\partial_t + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} \right) f(\mathbf{k}, \mathbf{r}, t) = (\partial_t f)_{\text{coll}}(\mathbf{k}, \mathbf{r}, t). \quad (264)$$

If scattering was absent (i.e., the right-hand side zero), the equation would simply be the continuity equation for $f(\mathbf{k}, \mathbf{r}, t)$ required by particle number conservation. Hence, all the magic is in the collision integral. For scattering off static potentials, it can be written as

$$(\partial_t f)_{\text{coll}}(\mathbf{k}, \mathbf{r}, t) = - \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \{ W(\mathbf{k}, \mathbf{k}') f(\mathbf{k}, \mathbf{r}, t) [1 - f(\mathbf{k}', \mathbf{r}, t)] - (\mathbf{k} \leftrightarrow \mathbf{k}') \}. \quad (265)$$

Here, $W(\mathbf{k}, \mathbf{k}')$ is the probability of a scattering process of a quasiparticle from momentum \mathbf{k} to \mathbf{k}' . The factors $f(\mathbf{k}, \mathbf{r}, t)$ and $[1 - f(\mathbf{k}', \mathbf{r}, t)]$ are the probability of there being a quasiparticle at \mathbf{k} that can be scattered in the first place and the probability of the state at

\mathbf{k}' being empty, respectively. The second term $\mathbf{k} \leftrightarrow \mathbf{k}'$ describes scattering *into* (as opposed to out of) the phase space volume near \mathbf{k} from a state at \mathbf{k}' and therefore comes with a negative sign. If a system has time-reversal symmetry, we have $W(\mathbf{k}, \mathbf{k}') = W(\mathbf{k}', \mathbf{k})$ and thus

$$(\partial_t f)_{\text{coll}}(\mathbf{k}, \mathbf{r}, t) = - \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} W(\mathbf{k}, \mathbf{k}') [f(\mathbf{k}, \mathbf{r}, t) - f(\mathbf{k}', \mathbf{r}, t)]. \quad (266)$$

An important approximation to make progress is the so-called *relaxation-time approximation*. We assume that the system is close to an equilibrium distribution $f_0(\mathbf{k}, \mathbf{r}, t)$, which is equal to the Fermi-Dirac distribution, but with a varying chemical potential $\mu(\mathbf{r}, t)$ and temperature $\beta(\mathbf{r}, t)$, which are the source of a position and time dependence in $f_0(\mathbf{k}, \mathbf{r}, t)$. The collision integral is then written using the ansatz

$$(\partial_t f)_{\text{coll}} = - \frac{f(\mathbf{k}, \mathbf{r}, t) - f_0(\mathbf{k}, \mathbf{r}, t)}{\tau(\epsilon_{\mathbf{k}})}, \quad (267)$$

i.e., we replace the integral with a simple linear function of $f(\mathbf{k}, \mathbf{r}, t)$ in the limit of small deviations from equilibrium. The quantity $\tau(\epsilon_{\mathbf{k}})$ is the relaxation time, quantifying the time scale of scattering events.

3. Conductivity

As a simple application of the Boltzmann theory using the relaxation time approximation, we compute the conductivity as a response to applying a small uniform electric field $\mathbf{E}(t)$. Then $f(\mathbf{k}, \mathbf{r}, t) = f(\mathbf{k}, t)$ is independent of \mathbf{r} . In absence of a magnetic field and for vanishing Berry curvature, the semiclassical equations of motion

$$\dot{\mathbf{r}} = \frac{\mathbf{k}}{m}, \quad \dot{\mathbf{k}} = -e\mathbf{E}, \quad (268)$$

allow to introduce the electric field in the Boltzmann equation (264). The applied electric field leads to a change $\delta f(\mathbf{k}, t)$ in the distribution $f(\mathbf{k}, t) = f_0(\mathbf{k}) + \delta f(\mathbf{k}, t)$. We can thus write the Boltzmann equation (264) to linear order in $\delta f(\mathbf{k}, t)$ and $\mathbf{E}(t)$ using their Fourier transforms

$$f(\mathbf{k}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\mathbf{k}, \omega) e^{-i\omega t}, \quad \mathbf{E}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathbf{E}(\omega) e^{-i\omega t}, \quad (269)$$

as

$$-i\omega \delta f(\mathbf{k}, \omega) - e\mathbf{E}(\omega) \cdot \nabla_{\mathbf{k}} f_0(\mathbf{k}) = - \frac{\delta f(\mathbf{k}, \omega)}{\tau(\epsilon_{\mathbf{k}})}. \quad (270)$$

This is an algebraic equation for $\delta f(\mathbf{k}, \omega)$ solved as

$$\delta f(\mathbf{k}, \omega) = \frac{e\tau(\epsilon_{\mathbf{k}})\mathbf{E}(\omega)}{1 - i\omega\tau(\epsilon_{\mathbf{k}})} \cdot \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}} \frac{\partial f_0(\epsilon)}{\partial \epsilon}. \quad (271)$$

Once we have obtained the distribution function, we can use it to calculate observables. For example, the quasiparticle current is given by

$$\mathbf{j}(\omega) = -2e \int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{v}_{\mathbf{k}} f(\mathbf{k}, \omega). \quad (272)$$

As an aside, were we interested in the thermal response of a material, we could instead compute the heat current

$$\mathbf{j}_h(\omega) = -2e \int \frac{d^3\mathbf{k}}{(2\pi)^3} \epsilon_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} f(\mathbf{k}, \omega). \quad (273)$$

For the case at hand, using $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$,

$$\mathbf{j}(\omega) = -\frac{e^2}{4\pi^3} \int d^3\mathbf{k} \frac{\tau(\epsilon_{\mathbf{k}})\mathbf{E}(\omega) \cdot \mathbf{v}_{\mathbf{k}}}{1 - i\omega\tau(\epsilon_{\mathbf{k}})} \frac{\partial f_0(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}}. \quad (274)$$

Comparing to Eq. (251), we find the conductivity

$$\sigma_{\alpha,\beta}(\omega) = -\frac{e^2}{4\pi^3} \int d\epsilon \frac{\partial f_0(\epsilon)}{\partial \epsilon} \frac{\tau(\epsilon)}{1 - i\omega\tau(\epsilon)} \int d\Omega_{\mathbf{k}} k^2 \frac{v_{\mathbf{k};\alpha} v_{\mathbf{k};\beta}}{|\mathbf{v}_{\mathbf{k}}|}. \quad (275)$$

We now discuss the result in different frequency regimes.

a. Limit of large frequencies If $\omega\tau \gg 1$ and for temperatures small compared to the Fermi energy, the energy integrand becomes a delta function multiplying i/ω . In the case of an isotropic system of mass m , we have $\sigma_{\alpha,\beta} = \delta_{\alpha,\beta}\sigma$ with

$$\begin{aligned} \sigma(\omega) &= i \frac{e^2}{4\pi^3 \omega} \int d\Omega_{\mathbf{k}} \frac{k_F}{m} k_{F,x}^2 \\ &= i \frac{e^2}{4\pi^3 \omega} \frac{k_F^3}{m} \frac{4\pi}{3} \\ &= i \frac{e^2 n}{m\omega} \\ &= i \frac{\omega_p^2}{4\pi\omega}, \end{aligned} \quad (276)$$

where $n = k_F^3/(3\pi^2)$ (spin degeneracy!). This agrees with our previous result Eq. (256).

b. Limit of small frequencies (dc limit) Before, our perfect conductor had a real delta function conductivity at small frequencies. Using the Boltzmann theory, we can obtain a

more realistic result in this limit, namely

$$\begin{aligned}\sigma(\omega) &= \frac{e^2 n}{m} \int d\epsilon \frac{\partial f_0(\epsilon)}{\partial \epsilon} \tau(\epsilon) \\ &= \frac{e^2 n \bar{\tau}}{m} \\ &= \frac{\omega_p^2 \bar{\tau}}{4\pi},\end{aligned}\tag{277}$$

where we simply defined the averaged relaxation time $\bar{\tau}$ as the integral with the derivative of the Fermi Dirac distribution, which is strongly peaked at the Fermi surface. This is the *Drude form* of the conductivity, which can also be derived with much more elementary means. Its important feature is that the conductivity is proportional to the relaxation time.

c. Limit of nearly constant relaxation times If the relaxation time depends only weakly on energy, we can use the approximation used to derive the Drude form also at finite frequencies to obtain

$$\begin{aligned}\sigma(\omega) &= \frac{\omega_p^2}{4\pi} \frac{\bar{\tau}}{1 - i\omega\bar{\tau}} \\ &= \frac{\omega_p^2}{4\pi} \frac{\bar{\tau}}{1 + \omega^2\bar{\tau}^2} + i \frac{\omega_p^2}{4\pi} \frac{\bar{\tau}^2\omega}{1 + \omega^2\bar{\tau}^2}.\end{aligned}\tag{278}$$

4. Optical properties

With the approximations above, there follows the dielectric function

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega} \frac{\bar{\tau}}{i + \omega\bar{\tau}}\tag{279}$$

directly from the conductivity. It is related to the complex index of refraction $n + i\kappa$ via $\epsilon = (n + i\kappa)^2$, which determines how light propagates inside the metal. Light with vacuum wave number $k = \omega/c$ has wave number $k(n + i\kappa)$ in the material. Hence, the penetration depth

$$\delta = c/(\omega\kappa)\tag{280}$$

determines how far light can penetrate the metal.

Straight-forward evaluation yields in the regime of small frequencies $\omega\bar{\tau} \ll 1 \ll \omega_p\bar{\tau}$ that

$$\delta(\omega) \approx \frac{c}{\omega_p} \sqrt{\frac{2}{\omega\bar{\tau}}},\tag{281}$$

yielding the dependence of the so-called skin depth of a metal $\delta \propto \omega^{-1/2}$.

For intermediate frequencies $1 \ll \omega\bar{\tau} \ll \omega_p\bar{\tau}$ the penetration depth is only weakly dependent on frequency as $\delta(\omega) \approx c/\omega_p$, which is in the range of hundreds Angstrom. (This regime does not include visible light.)

At ultraviolet frequencies $\omega \sim \omega_p$ the imaginary part of ϵ is very small yielding a strong increase in δ . The metal becomes transparent in the ultraviolet.

Note that we have only considered a single band model for a metal here. More discriminating optical properties, like the shiny colors of some metals like gold in the visible frequency range stem from interband transitions.

5. Computing the relaxation time

So far, we have introduced the relaxation time as a phenomenological function. We want to improve on that by considering actual scattering mechanisms now. We consider time-reversal invariant, isotropic, time-independent, and homogeneous systems, such that the relevant equation from the collision integral is

$$\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau(\epsilon_{\mathbf{k}})} = \int \frac{d^3\mathbf{k}'}{(2\pi)^3} W(\mathbf{k}, \mathbf{k}') [f(\mathbf{k}) - f(\mathbf{k}')]. \quad (282)$$

Let the only source of perturbation be an external electric field \mathbf{E} , such that

$$f(\mathbf{k}) = f_0(\mathbf{k}) + A(k) \mathbf{k} \cdot \mathbf{E} \quad (283)$$

to lowest order by isotropy. Then

$$f(\mathbf{k}) - f(\mathbf{k}') = A(k) (\mathbf{k} - \mathbf{k}') \cdot \mathbf{E} \quad (284)$$

because elastic scattering implies that $|\mathbf{k}| = |\mathbf{k}'|$. Let θ and θ' be the angles between \mathbf{E} and \mathbf{k} as well as between \mathbf{k}' and \mathbf{k} , respectively. Then $\mathbf{k}' \cdot \mathbf{E} = k' E (\cos \theta \cos \theta' + \sin \theta \sin \theta' \cos \phi')$, where ϕ' is the polar angle between \mathbf{k} and \mathbf{k}' . The latter term drops out of the integral by isotropy and

$$\begin{aligned} \frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau(\epsilon_{\mathbf{k}})} &= \frac{1}{(2\pi)^3} A(k) k E \cos \theta \int d\Omega_{\mathbf{k}'} (1 - \cos \theta') W(\mathbf{k}, \mathbf{k}') \\ &= \frac{1}{(2\pi)^3} [f(\mathbf{k}) - f_0(\mathbf{k})] \int d\Omega_{\mathbf{k}'} (1 - \cos \theta') W(\mathbf{k}, \mathbf{k}'). \end{aligned} \quad (285)$$

The relaxation time reduces to

$$\frac{1}{\tau(\epsilon_{\mathbf{k}})} = \int \frac{d^3\mathbf{k}'}{(2\pi)^3} (1 - \cos \theta') W(\mathbf{k}, \mathbf{k}'). \quad (286)$$

The factor $(1 - \cos \theta')$ gives more weight to the backscattering ($\theta' = \pi$) processes as compared to forward scattering ($\theta' = 0$).

a. Impurity scattering If we get microscopic information about an impurity potential \hat{V} , we can compute $W(\mathbf{k}, \mathbf{k}')$ by applying Fermi's golden rule

$$W(\mathbf{k}, \mathbf{k}') = 2\pi n_{\text{imp}} \left| \langle \mathbf{k} | \hat{V} | \mathbf{k}' \rangle \right|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}), \quad (287)$$

where n_{imp} is the density of impurities, which is assumed to be small enough from them to be considered as independent. Screened point charge scatterers of charge Ze have the potential

$$\langle \mathbf{k} | \hat{V} | \mathbf{k}' \rangle = \frac{4\pi Ze^2}{|\mathbf{k} - \mathbf{k}'|^2 + k_{\text{TF}}^2}. \quad (288)$$

In the limit of strong screening, $k_{\text{TF}} \gg k_{\text{F}}$, we can drop the $(\mathbf{k} - \mathbf{k}')$ in the matrix element and obtain

$$\begin{aligned} \frac{1}{\tau(\epsilon_{\text{k}})} &= 2\pi n_{\text{imp}} \left(\frac{4\pi Ze^2}{k_{\text{TF}}^2} \right)^2 \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} (1 - \cos \theta') \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) \\ &= \pi \nu(\epsilon_{\text{F}}) n_{\text{imp}} \left(\frac{4\pi Ze^2}{k_{\text{TF}}^2} \right)^2. \end{aligned} \quad (289)$$

This yields the temperature-independent *residual resistivity* of a metal

$$\rho = \frac{m}{e^2 n \tau(\epsilon_{\text{F}})}, \quad (290)$$

the ratio of which with the value of the resistivity at 300 K is the *residual resistance ratio* RRR, which is a measure for the amount of impurities in the system and hence a measure for sample quality. Typical values are in the tenths, clean materials reach RRR values in the thousands.

b. Electron-electron scattering The scattering rate between electrons is suppressed for energies close to the Fermi energy, because of the reduced phase space available for elastic scattering there. The life-time (here interpreted as the relaxation time) takes the form

$$\frac{1}{\tau(\epsilon)} = \frac{1}{\tau_e} \left(\frac{\epsilon}{\epsilon_{\text{F}}} \right)^2, \quad (291)$$

where τ_e is a constant and ϵ is measured with respect to the chemical potential, i.e., $\epsilon = 0$ at the Fermi level. Inserting this in the first line of Eq. (277) to compute $\bar{\tau}$, we find

$$\begin{aligned} \bar{\tau} &= \int d\epsilon \tau(\epsilon) \frac{\partial f_0}{\partial \epsilon} \\ &= \frac{\beta}{4} \int d\epsilon \frac{\tau(\epsilon)}{\cosh^2(\beta\epsilon/2)}. \end{aligned} \quad (292)$$

The latter integral is divergent for small ϵ .

In order to regulate it, we also consider coexisting impurity scattering. To show how one properly accounts for different scattering mechanisms we use *Matthiessen's rule*. It states that different independent scattering processes can be added at the level of the scattering rates, i.e.,

$$W(\mathbf{k}, \mathbf{k}') = W_1(\mathbf{k}, \mathbf{k}') + W_2(\mathbf{k}, \mathbf{k}'). \quad (293)$$

For the relaxation times and the resulting resistivity contributions this translates into

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2}, \quad \rho = \rho_1 + \rho_2. \quad (294)$$

It thus looks like we are coupling resistors in serial circuit. Matthiessen's rule can be inapplicable for 1D systems and if the τ 's are strongly \mathbf{k} -dependent.

Returning to our integral (292), we replace $1/\tau(\epsilon) = \epsilon^2/(\epsilon_F^2 \tau_e) + 1/\tau_0$, where τ_0 comes from impurity scattering

$$\begin{aligned} \bar{\tau} &\approx \frac{\beta}{4} \int d\epsilon \frac{1}{\cosh^2(\beta\epsilon/2)} \left(\tau_0 - \frac{\tau_0^2 \epsilon^2}{\tau_e \epsilon_F^2} \right) \\ &= \tau_0 - \frac{\pi^2}{3(\beta\epsilon_F)^2} \frac{\tau_0^2}{\tau_e}. \end{aligned} \quad (295)$$

The resistivity then becomes temperature dependent due to the electron-electron scattering as

$$\rho(T) = \rho_0 + \frac{\pi^2}{3} \frac{m}{ne^2\tau_E} \left(\frac{k_B T}{\epsilon_F} \right)^2. \quad (296)$$

The T^2 behavior is the main feature here which is often seen as an identification criterion for a Fermi liquid.

c. Sources of momentum loss Devil's advocate could argue at this point that if all scattering processes conserve momentum, no resistance should occur. This line of argumentation ignores the important role played by the lattice. In the case of electron-electron scattering, it also allows for *Umklapp processes* in the scattering for which

$$\mathbf{k} = \mathbf{k}' + \mathbf{G}, \quad (297)$$

where \mathbf{G} is a reciprocal lattice vector. Such a process leads to a static deformation of the lattice, which absorbs the momentum mismatch.

A second source of resistivity due to the lattice, which we have not touched upon is the scattering between electrons and phonons, i.e., elementary lattice vibrations. The resulting

relaxation time has the characteristic temperature dependence

$$\begin{aligned}\tau^{-1} &\propto \left(\frac{T}{\Theta_D}\right)^5, & T \ll \Theta_D, \\ \tau^{-1} &\propto \frac{T}{\Theta_D}, & T \gg \Theta_D,\end{aligned}\tag{298}$$

where the Debye temperature $k_B\Theta_D \approx c_s k_F$ with c_s the speed of sound.

D. Interacting instabilities

1. The fractional quantum Hall effect

We deduced that a 2D electron gas in a (strong) perpendicular magnetic field undergoes a dramatic spectral reorganization, where density of states is concentrated in highly degenerate Landau levels. The Hall conductivity $\sigma_{xy} = \nu e^2/h$ scales with the filling of the Landau levels ν . However, this result is at odds with the experimental observation of quantized values of the Hall conductivity $\sigma_{xy} = ne^2/h$ with $n \in \mathbb{Z}$. To reconcile theory and experiment, we had to account for the subtle role disorder plays in these systems: It broadens the Landau levels and leads to a quantization of the Hall conductivity by forming many localized states which do not contribute to transport. Only a single percolating state exists per Landau level which corresponds to the location of the jump in the Hall conductivity as a function of filling. Clearly, this noninteracting system is far away from the starting point of our discussion of Fermi liquids, for example. There is no well defined Fermi surface in momentum space. Moreover, many single-particle states are nearly degenerate in energy. It is thus imperative to ask how interactions can alter the nature of the ground state of a quantum Hall system.

It is the great achievement of Laughlin to propose a variational wavefunction without free parameters for the incompressible states that were observed experimentally at filling $\nu = 1/n$, with n an odd integer. We can construct the Laughlin wave function for N_p electrons in the following way for the disk geometry. The N_p -particle wave function for the *filled* lowest Landau level confined to a droplet of radius $\sqrt{2N_p}\ell$ is given by the single Slater determinant

$$\Psi_{\text{LLL}}(z_1, \dots, z_{N_p}) \propto \prod_{i < j}^{N_p} (z_i - z_j) \exp \left[- \sum_l^{N_p} |z_l|^2 / (4\ell^2) \right]. \tag{299}$$

The electron density per unit area inside the droplet is constant and given by $1/(2\pi\ell^2)$ By

raising the holomorphic part of the wave function to the power n

$$\Psi_n(z_1, \dots, z_{N_p}) \propto \prod_{i < j}^{N_p} (z_i - z_j)^n \exp \left[- \sum_l^{N_p} |z_l|^2 / (4\ell^2) \right], \quad (300)$$

one obtains the Laughlin wave function describing a droplet that

- has all electrons in the lowest Landau level due to the holomorphic structure
- covers an n -times larger area of radius $\sqrt{2n N_p} \ell$,
- is a featureless liquid with electron density reduced by a factor $1/n$,
- supports excitations of fractional charge e/n ,
- includes strong correlations between the electrons.

By inspection of the Laughlin wavefunction, one can gain some intuition as to why it might be an energetically favorable state for repulsively interacting electrons in the lowest Landau level. As any two electrons approach each other, the wavefunction has a n -th order zero, while the configurations with the electron positions well separated has the highest weight. Further, any two electrons with coordinates z_1 and z_2 have a relative angular momentum of $m^{\text{rel}} = n$ or higher. Here, the relative angular momentum of a two-particle state $(z_1 - z_2)^m$ is the exponent m . Remarkably, the elementary excitations are in some sense already contained in the analytic form of the Laughlin wavefunction. For example, the wavefunction of a quasi-hole with fractional charge $-e/n$ localized at z_0 is given by

$$\Psi_n^{\text{qh}}(z_1, \dots, z_{N_p} | z_0) \propto \Psi_n(z_1, \dots, z_{N_p}) \prod_l^{N_p} (z_0 - z_l). \quad (301)$$

As the Laughlin wave function is variational in nature, two immediate questions are: (i) How close is it to the actual ground state of the partially filled Landau level, when electrons are subject to Coulomb interactions? (ii) Does there exist a Hamiltonian for which Ψ_n is an incompressible ground state? The answer to (i) is given by numerical exact diagonalization studies of finite systems, which showed that the Laughlin state is in the same universality class as the exact ground state, the so-called Coulomb ground state. The answer to (ii) will be given in this and the following section.

Trugman and Kivelson showed how to construct a Hamiltonian for which Ψ_n is an exact and unique zero-energy ground state. Crucial to their derivation is the fact that any two particles have relative angular momentum $m^{\text{rel}} = n$ or higher in the Laughlin wave function. As an immediate consequence, Ψ_n is annihilated by the projector on states with angular momentum $m^{\text{rel}} < n$. This projector is precisely the so-called pseudopotential Hamiltonian that they propose. In configuration space, its matrix elements are derivatives of delta-functions. Physically, it corresponds to a highly local repulsive interaction.

2. Superconductivity

The theory of superconductivity is a very rich field, and as a result we can only give a very short account of the theoretical description of superconductors. We will focus on the derivation of the superconducting ground state and its elementary excitations.

Many materials turn superconducting at low temperatures (ironically, many noble metals and the excellent conductor copper don't). The phenomenology of the superconducting state is two-fold: (1) The resistivity of a superconductor vanishes exactly. (2) The magnetic field is expelled from the bulk of a superconductor (or channelled in very thin flux tubes in so-called type-II superconductors). The latter is called the Meissner-effect. Only the combination of properties (1) and (2) yield a well-defined thermodynamic state. It also implies the existence of persistent currents in a superconductor, which do not decay.

a. Cooper pairs The elementary building block of superconductors are Cooper pairs, that is, coherent combinations of two-electron states. The formation of Cooper pairs results from some effective attractive interaction between electrons, which overcomes their repulsive Coulomb interaction. In so-called conventional superconductors, this attractive interaction is mediated by phonons (lattice distortions). An electron passing through the crystal leaves behind a slowly relaxing lattice distortion (the slowness is determined by the large mass ratio M_{ion}/m of the ionic and electronic mass). This polarized crystal environment is seen by the other electron of the Cooper pair as an attracting force.

Here, we do not detail the phononic origin of the interaction and simply assume that there exists some attractive interaction between electrons. To understand the formation of

Cooper pairs more quantitatively, we consider the following wave function ansatz

$$|\Psi_{12}(\mathbf{K})\rangle = \sum_{\mathbf{k}, \sigma, \sigma'} a_{\mathbf{k}, \sigma, \sigma'} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{-\mathbf{k} + \mathbf{K}, \sigma'}^\dagger |0\rangle, \quad (302)$$

which describes two electrons (\mathbf{k}, σ) and $(\mathbf{K} - \mathbf{k}, \sigma')$ added to the filled Fermi sea ground state $|0\rangle$. Since we expect the system to remain translationally invariant, we have assigned a well-defined momentum \mathbf{K} to this state. Anticipating a minimization of the energy of this state, we can further refine this ansatz. We assume that attractive interactions exist between electrons only in a small energy range ω , which for the case of phonons can be taken as the Debye frequency of the material, i.e., if $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{K} - \mathbf{k}}| \leq \omega$. Figure 7 a) suggests that most electron pairs can take advantage of this interaction if $\mathbf{K} = 0$. We furthermore assume that the ground state in this two-electrons-above-the-Fermi-sea subspace has even orbital character (as is usually the case for symmetric attractive potentials). To obtain a valid fermionic two-body wave function (which is antisymmetric under particle exchange), we thus have to make the spin part antisymmetric, i.e., the two electrons in our ansatz have opposite spin, yielding

$$|\Psi_{12}\rangle = \sum_{\mathbf{k}} a_{\mathbf{k}} \hat{c}_{\mathbf{k}, \uparrow}^\dagger \hat{c}_{-\mathbf{k}, \downarrow}^\dagger |0\rangle. \quad (303)$$

We want to study this family of states subject to the Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} - \frac{V}{2} \sum'_{\mathbf{k}, \mathbf{q}, \sigma} \hat{c}_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger \hat{c}_{-\mathbf{k} - \mathbf{q}, -\sigma}^\dagger \hat{c}_{-\mathbf{k}, -\sigma} \hat{c}_{\mathbf{k}, \sigma} \quad (304)$$

where we take $V \neq 0$ only for $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{K} - \mathbf{k}}| \leq \omega$, which is indicated by the primed sum. Notice also that we have already restricted the interaction to the so-called ‘Cooper channel’, i.e., we have dropped all terms of a generic translation symmetry preserving interaction that do not connect states of the form (303). The energy is given by

$$\begin{aligned} E &= \langle \Psi_{12} | \hat{H} | \Psi_{12} \rangle \\ &= 2 \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |a_{\mathbf{k}}|^2 - V \sum'_{\mathbf{k}, \mathbf{q}} a_{\mathbf{k} + \mathbf{q}}^* a_{\mathbf{k}}. \end{aligned} \quad (305)$$

We minimize it subject to the constraint $\sum_{\mathbf{k}} |a_{\mathbf{k}}|^2 = 1$,

$$\frac{\partial}{\partial a_{\mathbf{k}}^*} \left(E - \lambda \sum_{\mathbf{k}} |a_{\mathbf{k}}|^2 \right) \quad (306)$$

yielding

$$(2\epsilon_{\mathbf{k}} - \lambda) a_{\mathbf{k}} = V \sum'_{\mathbf{k}'} a_{\mathbf{k}'}. \quad (307)$$

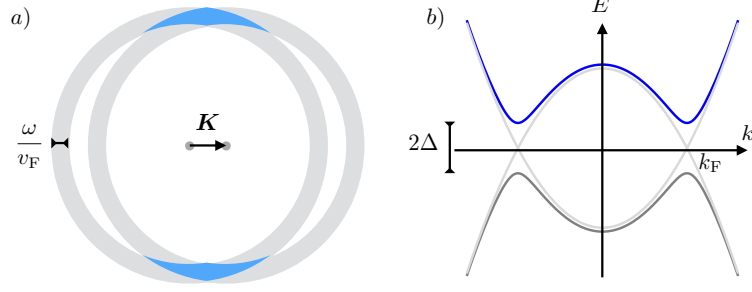


Figure 7. a) Areas in momentum space in which quasiparticles can interact when forming Cooper pairs with center of mass momentum \mathbf{K} are marked in blue. The largest contribution is obtained for $\mathbf{K} = 0$. b) Excitation spectrum (blue) of the Bogoliubov quasiparticles in a superconductor.

Dividing Eq. (307) by $(2\epsilon_{\mathbf{k}} - \lambda)$, summing both sides over \mathbf{k} (with a primed sum), we can shorten $\sum'_{\mathbf{k}'} a_{\mathbf{k}'}$ and obtain

$$1 = V \sum'_{\mathbf{k}'} \frac{1}{2\epsilon_{\mathbf{k}'} - \lambda}. \quad (308)$$

Multiplying the complex conjugate of Eq. (307) by $a_{\mathbf{k}}$ and summing over \mathbf{k} , we obtain

$$2 \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |a_{\mathbf{k}}|^2 - \lambda = V \sum'_{\mathbf{k}', \mathbf{k}} a_{\mathbf{k}'}^* a_{\mathbf{k}}, \quad (309)$$

which, when compared with Eq. (305) gives $\lambda = E$. Thus,

$$1 = V \sum'_{\mathbf{k}'} \frac{1}{2\epsilon_{\mathbf{k}'} - E} = V \int_0^{\omega} d\epsilon \frac{\nu(\epsilon)}{2\epsilon - E}. \quad (310)$$

Setting $\nu(\epsilon) \approx \nu(\epsilon_F)$, we can compute the integral and obtain

$$\begin{aligned} E &= - \frac{2\omega \exp\left(-\frac{2}{\nu(\epsilon_F)V}\right)}{1 - \exp\left(-\frac{2}{\nu(\epsilon_F)V}\right)} \\ &\approx - 2\omega e^{-2/[\nu(\epsilon_F)V]}. \end{aligned} \quad (311)$$

The two main features of this result are (1) the negative sign, indicating that it is indeed energetically favorable to form Cooper pairs, and (2) the energy gain is exponential in the product of interaction strength and density of states. One can show that even if the ansatz is less restrictive than ours, this is the solution minimizing the energy of the model.

b. Superconducting ground state In the next step we want to find the ground state of the Hamiltonian (304), i.e., minimize it over the full fermionic Fock space instead of

the two-particle excitation state considered so far. Implicitly, we will perform a mean-field approximation for the case of small interaction V . We start out with a completely trivial rewriting of the fermionic creation and annihilation operators into new linear combinations as

$$\begin{aligned}
\alpha_{\mathbf{k}} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k},\uparrow} - v_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow}^\dagger, \\
\alpha_{-\mathbf{k}} &= u_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow} + v_{\mathbf{k}} \hat{c}_{\mathbf{k},\uparrow}^\dagger, \\
\alpha_{\mathbf{k}}^\dagger &= u_{\mathbf{k}} \hat{c}_{\mathbf{k},\uparrow}^\dagger - v_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow}, \\
\alpha_{-\mathbf{k}}^\dagger &= u_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow}^\dagger + v_{\mathbf{k}} \hat{c}_{\mathbf{k},\uparrow},
\end{aligned} \tag{312}$$

where we have introduced the real (and \mathbf{k} even) functions $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. Their reality is merely a gauge fixing. We have also explicitly locked the sign of \mathbf{k} in α to the spin degree of freedom. One verifies that the $\alpha_{\mathbf{k}}$ obey the usual fermionic anticommutation relations if

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1, \tag{313}$$

which shall be imposed from here on.

Let us rewrite the Hamiltonian in the new operators. We start with the noninteracting part

$$\begin{aligned}
\hat{H}_0 &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k},\sigma}^\dagger \hat{c}_{\mathbf{k},\sigma} \\
&= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (\hat{c}_{\mathbf{k},\uparrow}^\dagger \hat{c}_{\mathbf{k},\uparrow} + \hat{c}_{-\mathbf{k},\downarrow}^\dagger \hat{c}_{-\mathbf{k},\downarrow}) \\
&= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} [2v_{\mathbf{k}}^2 + (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2)(\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}}) + 2u_{\mathbf{k}} v_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{-\mathbf{k}}^\dagger + \alpha_{-\mathbf{k}} \alpha_{\mathbf{k}})].
\end{aligned} \tag{314}$$

The interacting part gives

$$\begin{aligned}
\hat{H}_{\text{int}} &= -\frac{V}{2} \sum'_{\mathbf{k},\mathbf{q},\sigma} \hat{c}_{\mathbf{k}+\mathbf{q},\sigma}^\dagger \hat{c}_{-\mathbf{k}-\mathbf{q},-\sigma}^\dagger \hat{c}_{-\mathbf{k},-\sigma} \hat{c}_{\mathbf{k},\sigma} \\
&= -V \sum'_{\mathbf{k},\mathbf{k}'} \hat{c}_{\mathbf{k}',\uparrow}^\dagger \hat{c}_{-\mathbf{k}',\downarrow}^\dagger \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow} \\
&= -V \sum'_{\mathbf{k},\mathbf{k}'} [u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} (1 - \alpha_{-\mathbf{k}'}^\dagger \alpha_{-\mathbf{k}'} - \alpha_{\mathbf{k}'}^\dagger \alpha_{\mathbf{k}'}) (1 - \alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}} - \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}) \\
&\quad + (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) u_{\mathbf{k}'} v_{\mathbf{k}'} (1 - \alpha_{-\mathbf{k}'}^\dagger \alpha_{-\mathbf{k}'} - \alpha_{\mathbf{k}'}^\dagger \alpha_{\mathbf{k}'}) (\alpha_{-\mathbf{k}} \alpha_{\mathbf{k}} + \alpha_{\mathbf{k}}^\dagger \alpha_{-\mathbf{k}}^\dagger) \\
&\quad + (\text{more forth-order terms in } \alpha)].
\end{aligned} \tag{315}$$

To proceed, we first neglect the residual terms of fourth order in α . This seems arbitrary and highlights a general problem of mean-field approximations: If the ansatz (in this case

the expressions for the α s) is not a good description of the physics, we have no chance of proceeding in a controlled way. The other problem are terms quadratic in the α s but of the form $\alpha^\dagger \alpha^\dagger$ or the hermitian conjugate. What our mean-field solution needs to achieve is that all these terms (or better put, their prefactors) vanish. Notice that such terms appear both in \hat{H}_0 and in \hat{H}_{int} . The prefactor of terms of this form is

$$2\epsilon_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} - V(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) \sum'_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}. \quad (316)$$

To have it vanish, we sum over (the primed set of) \mathbf{k} and set $\sum'_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} = \Delta/V$ (thereby defining the constant Δ). This yields

$$2\epsilon_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} = \Delta(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2), \quad (317)$$

which has the normalized solution

$$u_{\mathbf{k}}^2 = \frac{1 + \xi_{\mathbf{k}}}{2}, \quad v_{\mathbf{k}}^2 = \frac{1 - \xi_{\mathbf{k}}}{2}, \quad \xi_{\mathbf{k}} = \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \quad (318)$$

The transformation from \hat{c} operators to the α operators is called a Bogoliubov transformation. Finally, to calculate Δ from this, we start from its definition

$$\begin{aligned} \Delta &= V \sum'_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \\ &= \frac{V}{2} \sum'_{\mathbf{k}} \sqrt{1 - \xi_{\mathbf{k}}^2} \\ &= \frac{V}{2} \sum'_{\mathbf{k}} \frac{\Delta}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \end{aligned} \quad (319)$$

Dividing it out and going to an integral representation

$$\begin{aligned} 1 &= \frac{V}{4} \int_{-\omega}^{\omega} d\epsilon \frac{\nu(\epsilon)}{\sqrt{\epsilon^2 + \Delta^2}} \\ &\approx \frac{V\nu(\epsilon_F)}{4} \int_{-\omega}^{\omega} d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}}, \end{aligned} \quad (320)$$

yields a solvable integral that

$$\Delta = 2\omega e^{-2/[\nu(\epsilon_F)V]}. \quad (321)$$

With the off-diagonal terms vanishing, the total Hamiltonian, omitting the fourth order terms is of the form

$$\begin{aligned} \hat{H}_0 + \hat{H}_{\text{int}} &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} 2v_{\mathbf{k}}^2 - V \sum'_{\mathbf{k}, \mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \\ &\quad + \sum_{\mathbf{k}} \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} (\alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}} + \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}). \end{aligned} \quad (322)$$

Let us first take a closer look at the constant terms, which encode the shift in ground state energy. With the help of some more, less interesting integrals one can compute them in the limit of small Δ as

$$- \nu(\epsilon_F) \Delta^2/4. \quad (323)$$

Again the main feature of this expression is its negative sign, signaling that our mean-field state is indeed lower in energy than the noninteracting Fermi sea. It is the condensation energy of the superconducting state.

The second line in Eq. (322) is the Hamiltonian for a noninteracting Fermi liquid with only manifestly positive energies. The ground state is thus the state annihilated by all $\alpha_{\mathbf{k}}$ and $\alpha_{-\mathbf{k}}$ operators. However, we should not forget that these operators are superpositions of electron creation and annihilation operators. A first guess would be to write the ground state as

$$\begin{aligned} |\tilde{0}\rangle &= \prod_{\mathbf{k}} \alpha_{\mathbf{k}} \alpha_{-\mathbf{k}} |\text{vac}\rangle \\ &= \prod_{\mathbf{k}} (u_{\mathbf{k}} v_{\mathbf{k}} + v_{\mathbf{k}}^2 \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{-\mathbf{k}}^\dagger) |\text{vac}\rangle. \end{aligned} \quad (324)$$

This state is not normalized, though. The properly normalized state is

$$|0\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{-\mathbf{k}}^\dagger) |\text{vac}\rangle. \quad (325)$$

This many-body state has no definite particle number. The particle number conservation is spontaneously broken in a superconductor: The condensate can absorb and emit Cooper pairs.

c. Excitations The elementary excitations above this ground state can be directly read off thanks to the noninteracting structure of the mean-field Hamiltonian. The quasiparticles created by the $\alpha_{\mathbf{k}}^\dagger$ operators, called Bogoliubons, are fundamentally different from the quasiparticles in a Fermi liquid in that they create a coherent superposition of a particle and a hole. The $u_{\mathbf{k}}$ gives the particle-like weight and the $v_{\mathbf{k}}$ gives the hole-like weight. Far away from the Fermi surface, they tend to $v_{\mathbf{k}} \rightarrow 1$ and $u_{\mathbf{k}} \rightarrow 0$ inside the Fermi sea, while the opposite happens far outside the Fermi sea. Right at the Fermi surface they are an equal amplitude superposition of electron and hole. The spectrum of these single-particle like excitations

$$\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \quad (326)$$

is gapped, i.e., the smallest excitation above the ground state has energy gap 2Δ . [See Fig. 7 b).]

From this observation, we can conclude that the superconductor must support persistent currents. We can view a state which carries a current \mathbf{j} in momentum space as displacing the Fermi sea by an amount proportional to the current strength. After switching off the electric field that drove the current, elastic scattering processes from one side of the displaced Fermi sea to the opposite side (at impurities, phonons, etc.) lead to a relaxation of the Fermi sea to its original form. If, however, there is an excitation gap 2Δ and the displacement of the Fermi sea is small enough such that none of the states on the left end of the displaced Fermi sea has an energy of 2Δ or more above the energy of any state on the right side of the displaced Fermi sea, no such elastic scattering is possible. We can be more quantitative by considering a displacement of the Fermi sphere

$$\delta\mathbf{k} = -m\delta\mathbf{v} = \frac{m}{ne}\mathbf{j}. \quad (327)$$

Elastic scattering processes require

$$\frac{(k_F + \delta k)^2}{2m} - \frac{(k_F - \delta k)^2}{2m} \geq 2\Delta. \quad (328)$$

From this, we can deduce the critical current density above which the superconductivity breaks down as

$$j_{\text{crit}} = \frac{2en\Delta}{k_F}. \quad (329)$$

Inserting typical values, we get $j_{\text{crit}} \sim 10^7$ A/cm², which is a pretty sizable value.

3. Density waves

We found in our mean-field analysis of the superconductor that the ground state breaks spontaneously the particle number conservation, which can be seen from

$$\langle 0 | \hat{c}_{\mathbf{k},\uparrow}^\dagger \hat{c}_{-\mathbf{k},\downarrow}^\dagger | 0 \rangle = \frac{1}{2} \frac{\Delta}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \quad (330)$$

Here we want to think about systems with ground states that instead break translation symmetry, but conserve particle number. These charge density waves have nonvanishing ground state expectation values for operators of the form (we neglect the spin degree of

freedom in this section)

$$\langle 0 | \hat{c}_{\mathbf{k}-\mathbf{Q}/2}^\dagger \hat{c}_{\mathbf{k}+\mathbf{Q}/2} | 0 \rangle = \frac{1}{2} \frac{\Delta_{\mathbf{k},\mathbf{Q}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k},\mathbf{Q}}^2}}. \quad (331)$$

In writing Eq. (331), we have introduced a much more general order parameter than for the superconducting case: First, it depends on the variational parameter \mathbf{Q} , the center of mass momentum of the density wave. A density wave has only \mathbf{Q} and $-\mathbf{Q}$ contributions for one specific \mathbf{Q} . Second, we have allowed for a dependence of the order parameter on the relative momentum \mathbf{k} of the electrons that form the density wave. If we Fourier transform this order parameter in real space, we find a charge density modulation

$$\Delta_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{Q}\cdot\mathbf{r}} \Delta_{\mathbf{k},\mathbf{Q}} + e^{-i\mathbf{Q}\cdot\mathbf{r}} \Delta_{\mathbf{k},-\mathbf{Q}} \quad (332)$$

As with superconductivity, a density wave state is brought about by interactions. If these are small, charge density waves are typically driven by *nesting* features of the Fermi surface. If one displaces the Fermi surface by \mathbf{Q} , it overlaps to a large extent with other parts of the Fermi surface. For concreteness, consider a two-band model with equal dispersions that are shifted with respect to one another in momentum space and have opposite sign (i.e., one is electron-like and one is hole like)

$$\begin{aligned} \hat{H}_0 &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}-\mathbf{Q}/2} \hat{c}_{\mathbf{k},+}^\dagger \hat{c}_{\mathbf{k},+} - \sum_{\mathbf{k}} \epsilon_{\mathbf{k}+\mathbf{Q}/2} \hat{c}_{\mathbf{k},-}^\dagger \hat{c}_{\mathbf{k},-} \\ &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \left(\hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^\dagger \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+} - \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^\dagger \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-} \right), \end{aligned} \quad (333)$$

where $\hat{c}_{\mathbf{k},\pm}^\dagger$ are the electronic creation operators of the \pm bands. As before, we take the liberty of restricting the interaction to the desired channel

$$\hat{H}_{\text{int}} = -\frac{V}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma}' \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^\dagger \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-} \hat{c}_{\mathbf{k}'-\mathbf{Q}/2,-}^\dagger \hat{c}_{\mathbf{k}'+\mathbf{Q}/2,+} \quad (334)$$

Upon the replacement

$$\begin{aligned} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^\dagger &\rightarrow \hat{c}_{\mathbf{k},\uparrow}^\dagger \\ \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+} &\rightarrow \hat{c}_{\mathbf{k},\uparrow} \\ \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^\dagger &\rightarrow \hat{c}_{-\mathbf{k},\downarrow}^\dagger \\ \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-} &\rightarrow \hat{c}_{-\mathbf{k},\downarrow} \end{aligned} \quad (335)$$

this problem is completely equivalent to the superconducting Hamiltonian that we studied before. Thus, the ansatz

$$\begin{aligned}
\alpha_{\mathbf{k}} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+} - v_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}, \\
\alpha_{-\mathbf{k}} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^{\dagger} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^{\dagger}, \\
\alpha_{\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^{\dagger} - v_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^{\dagger}, \\
\alpha_{-\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^{\dagger} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^{\dagger},
\end{aligned} \tag{336}$$

will deliver a mean-field solution. Notice that these operators are made of either creation or annihilation operators, but not a superposition of both, reflecting the intact particle number conservation. On the other hand, they are a superposition of operators with \mathbf{k} and $\mathbf{k} + \mathbf{Q}$, reflecting the broken translation symmetry. We conclude that our simple model for a charge density wave has a fully gapped ground state, while it had an electron and a hole-like Fermi pocket initially. Notice also that the interaction (334) is actually a repulsive interaction, because bringing it to a density-density form $\hat{c}_{\mathbf{k}+\mathbf{Q}/2,+}^{\dagger} \hat{c}_{\mathbf{k}'+\mathbf{Q}/2,+} + \hat{c}_{\mathbf{k}'-\mathbf{Q}/2,-}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}$ requires one anticommutation.

The mean-field charge density wave state has a nonvanishing expectation value for

$$\langle 0 | \hat{c}_{\mathbf{k}-\mathbf{Q}/2,-}^{\dagger} \hat{c}_{\mathbf{k}+\mathbf{Q}/2,+} | 0 \rangle = \frac{1}{2} \frac{\Delta_{\mathbf{Q}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{Q}}^2}} \tag{337}$$

and behaves like a band insulator as far as transport properties are concerned (albeit with a much smaller gap). Let us finally comment on the possible \mathbf{k} dependence of the gap introduced in Eq. (331). This feature can be found both in superconductors and in density wave states, but it requires a different interaction potential to be realized. If the interaction potential penalizes the $l = 0$ mode (thinking about an expansion of a rotationally symmetric potential in spherical harmonics), for example by being repulsive on short distances in the case of a superconductor, the ground state may be found in a higher angular momentum channel. The conventional states that we discussed here, with \mathbf{k} -independent order parameter, correspond to the $l = 0$ or s -wave case. Higher angular momentum cases such as p -wave and d -wave (the cuprate superconductors) are of high practical relevance as well and show some unique features. To be more precise, since the crystal breaks rotational symmetry, the symmetry-breaking order parameters should better be classified by the irreducible representations of the point group, rather than by angular momenta.

4. Mott insulators

With the exception of the (fractional) quantum Hall effect, we have considered models which have weak interactions and where a description in momentum space was most convenient and appropriate. In this section, we will be concerned with the paradigmatic Hubbard model, which is very important in the theoretical study of cuprate superconductors. The Hubbard model forces us to take a different angle on the problem: It involves comparably strong interactions and the lattice plays a crucial role. In some regimes a configuration space picture is more practical, in others we will work in momentum space.

Simple theoretical models are often introduced because they illustrate a physical effect while being exactly soluble. The Hubbard model is a very different case. Neither is it analytically soluble, nor have numerical approaches been successful in establishing its ground state properties. The numerical investigation of the Hubbard model is still an active area of condensed matter research.

The story of the Hubbard model will consist of a charge and a spin part. We relegate the spin part to the next chapter, where we study magnetic instabilities of matter.

The charge degrees of freedom of the Hubbard model feature a *metal-insulator transition*. The interesting side of this will be the insulator, which is termed a *Mott insulator*. So far, we have mostly been talking about (true or mean-field induced) band insulators (with the exception of the fractional quantum Hall effect). The Mott insulator, in contrast, is interaction induced but does not allow for a band insulator description. Furthermore, it does not break any symmetries of the system spontaneously.

The Hubbard model defined on a square lattice, with one (spinful) orbital per site is defined, within a tight-binding approximation, by the Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \quad (338)$$

where the first sum runs over directed nearest-neighbor links on the lattice and the density operators are defined as $\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$. We will study the model at half filling, i.e., in a Hilbert space with as many electrons as there are lattice sites (filling 1 would be twice as many electrons, as we can put an up-spin and a down-spin electron on each site). There are two obvious limits of the model:

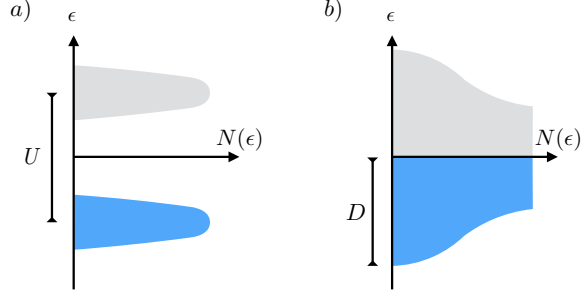


Figure 8. Density of states of the 3D Hubbard model a) in the limit $U \gg t$ displaying the lower and upper Hubbard band and b) in the metallic band limit $U = 0$.

a. Metallic limit For $U = 0$ the Hamiltonian reduces to

$$\hat{H}_{U=0} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^{\dagger} \hat{c}_{\mathbf{k}, \sigma} \quad (339)$$

with dispersion

$$\epsilon_{\mathbf{k}} = -2t (\cos k_x + \cos k_y + \cos k_z). \quad (340)$$

and the unique ground state

$$|\Psi_{U=0}\rangle = \prod_{\mathbf{k}} \Theta(-\epsilon_{\mathbf{k}}) \hat{c}_{\mathbf{k}, \uparrow}^{\dagger} \hat{c}_{\mathbf{k}, \downarrow}^{\dagger} |0\rangle. \quad (341)$$

We now wrote the model in 3D, where the van Hove point that we encountered in 2D is not a singularity in the density of states. The bandwidth $2D = 12t$ in 3D. To study the state at small but finite U is challenging and there are no controlled approximations available. An instructive variational approach is the *Gutzwiller approximation*. We define the following densities

1 electron density

s_{\uparrow} density of singly occupied lattice sites with spin \uparrow

s_{\downarrow} density of singly occupied lattice sites with spin \downarrow

d density of doubly occupied sites

h density of empty sites

Not all of these quantities are independent. The following relations must be satisfied

$$h = d, \quad s_{\downarrow} = s_{\uparrow} \equiv \frac{s}{2}, \quad 1 = s + 2d. \quad (342)$$

The classical energy (density) cost due to the interaction is given by Ud .

The Gutzwiller approximation includes correlation effects by renormalizing hopping probabilities in a statistically average setting. We focus on hopping processes that keep the density of doubly occupied sites constant (and with it the interaction energy Ud). Let's first consider a hopping process from a singly occupied site (i) to an empty site (j). The hopping probability depends on the availability of the initial configuration. Let $P_0(\uparrow_i, 0_j)/P_0(\downarrow_i, 0_j)$ be these probabilities to find the initial state in absence of interactions. We relate it to the renormalized probabilities $P(\uparrow_i, 0_j)/P(\downarrow_i, 0_j)$ via a factor g_t as

$$P(\uparrow_i, 0_j) + P(\downarrow_i, 0_j) = g_t[P_0(\uparrow_i, 0_j) + P_0(\downarrow_i, 0_j)]. \quad (343)$$

We thus have

$$P(\uparrow_i, 0_j) + P(\downarrow_i, 0_j) = sh = sd = (1 - 2d)d. \quad (344)$$

In absence of correlations, this probability can be computed explicitly

$$P_0(\uparrow_i, 0_j) = n_{i,\uparrow}(1 - n_{i,\downarrow})(1 - n_{j,\uparrow})(1 - n_{j,\downarrow}) = \frac{1}{16}, \quad (345)$$

and similarly for \downarrow . We can now compute

$$g_t = 8d(1 - 2d). \quad (346)$$

The other hopping processes that leave d constant are $(\uparrow\downarrow, \uparrow) \rightarrow (\uparrow, \uparrow\downarrow)$, as well as the one with spin reversed. One finds the same renormalization factor $g_t = 8d(1 - 2d)$ for these processes. We do not consider processes of the form $(\uparrow\downarrow, 0) \rightarrow (\uparrow, \downarrow)$ that change d . The factor g_t is used to renormalize the hopping probability, i.e., $t \rightarrow g_t t$. We thus find the energy of a sector of constant d to be

$$E(d) = g_t \epsilon_{\text{kin}} + Ud, \quad \epsilon_{\text{kin}} = \frac{1}{N} \int_{-D}^0 d\epsilon \nu(\epsilon) \epsilon. \quad (347)$$

Note that this is not a variational calculation in a strict sense, as $E(d)$ is not guaranteed to be an upper bound to the ground state energy. Nevertheless, we can minimize $E(d)$ with respect to d and obtain

$$d = \frac{1}{4} \left(1 - \frac{U}{U_c} \right), \quad g_t = 1 - \left(\frac{U}{U_c} \right)^2 \quad (348)$$

with

$$U_c = 8|\epsilon_{\text{kin}}| \approx 25t \approx 4D. \quad (349)$$

The theory thus naturally produces a critical interaction strength, and for $U > U_c$ double occupancy and with it any hopping is completely suppressed. This provides a qualitative description for the metal-insulator transition in a Mott insulator. Obvious shortcomings are that only local correlations are included to renormalize parameters, as opposed to correlations between different lattice sites, and the spin degree of freedom plays no role in this treatment.

We can argue more precisely why the system turns insulating by splitting up the conductivity into two parts that correspond to different d sectors. Using the conductivity from Eq. (258), we write

$$\text{Re } \sigma(\omega) = \frac{\omega_p^{\star 2}}{4} \delta(\omega) + \text{Re } \sigma^{\text{high energy}}(\omega), \quad (350)$$

where the first term is the conductivity associated with the Hamiltonian

$$\hat{H}_{\text{ren}} = \sum_{\mathbf{k}, \sigma} g_t \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} + U d \quad (351)$$

while the second part corresponds to sectors with at least one more doubly occupied site. Since $\omega_p^2 \propto 1/m$, it renormalizes as $\omega_p^{\star 2} = g_t \omega_p^2$. We can now make use of the f sum rule (259)

$$\int_0^\infty d\omega \text{Re } \sigma(\omega) = \frac{\omega_p^2}{8} g_t + I_{\text{high energy}} = \frac{\omega_p^2}{8}. \quad (352)$$

According to Eq. (348), the weight of the low energy contribution vanishes as $U \rightarrow U_c$, and the f sum rule dictates that it is sifted to the high-energy contribution (i.e., to large ω). The system becomes insulating.

b. Insulating limit For $t = 0$, the ground state with zero energy has exactly one electron per site. However, this ground state is not unique due to the spin degree of freedom. In fact, any state of the form

$$|\Psi\{\sigma_i\}\rangle = \prod_i \hat{c}_{i, \sigma_i}^\dagger |0\rangle \quad (353)$$

with any spin configuration $\{\sigma_i\}$ is a ground state. The ground state degeneracy is 2^N . It is therefore a bit dangerous to call this an insulator, without knowing how this degeneracy is lifted by small perturbations. However, since all these ground states do not differ in the occupation numbers of each site, we can already anticipate that no electric transport will be possible no matter how the degeneracy is lifted. The lifting of the ground state degeneracy by small t will be the subject of the spin part of the Hubbard model story contained in

the next chapter. Excited states at energy U feature exactly one empty and one doubly occupied site.

We now slightly depart from the limit $t = 0$ and consider the insulating state with $t \ll U$. The excitations of one site being doubly occupied and one site being empty are called *doublon* and *holon*, respectively. When t is finite, these excitations can actually hop and move through the lattice. This lifts some of the degeneracy of the “excited band” and gives a dispersion

$$E_{\mathbf{k},\mathbf{k}'} = U + \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}'} > U - 12t. \quad (354)$$

Upon increasing t , the two sectors (i.e., the ground state sector and this doublon-holon band) start to overlap. When not overlapping, the two bands are called the lower and upper Hubbard band. [See Fig. 8 a).] A holon is a hole in the lower Hubbard band and a doublon is a particle in the upper Hubbard band. This density of states structure (there are no actual energy bands here, the name is a complete abuse of language) is called a Mott insulator. The gap is entirely due to the interaction, without the need for any mean-field treatment or the like. It is therefore fundamentally different from the band insulators that we considered before. We should keep in mind that we have neglected the role played by the spin.

c. The metallic state as a Fermi liquid In the uncorrelated case, we have

$$\epsilon_{\text{kin}} = \frac{1}{N} \sum_{\mathbf{k} \in \text{FS}} \epsilon_{\mathbf{k}}. \quad (355)$$

Within the Gutzwiller we found $\epsilon_{\text{kin}} \rightarrow g_t \epsilon_{\text{kin}}$. One can furthermore show (we don’t give a proof here) that within the same approximation a finite interaction strength induces a nonzero and constant occupation number n_{out} outside the Fermi surface while at the same time the density inside the Fermi surface n_{in} is reduced below 1 but remains constant. The total must correspond to the filling, i.e.,

$$\frac{1}{2} = \frac{1}{N} \sum_{\mathbf{k} \in \text{FS}} n_{\text{in}} + \frac{1}{N} \sum_{\mathbf{k} \notin \text{FS}} n_{\text{out}} = \frac{n_{\text{in}} + n_{\text{out}}}{2}, \quad (356)$$

where we used that the Fermi sea and its complement are equal in size. This gives the constraint

$$g_t \epsilon_{\text{kin}} = \frac{1}{N} \sum_{\mathbf{k} \in \text{FS}} n_{\text{in}} \epsilon_{\mathbf{k}} + \frac{1}{N} \sum_{\mathbf{k} \notin \text{FS}} n_{\text{out}} \epsilon_{\mathbf{k}}. \quad (357)$$

We can furthermore use the particle-hole symmetry of the band structure

$$\sum_{\mathbf{k} \in \text{FS}} \epsilon_{\mathbf{k}} = - \sum_{\mathbf{k} \notin \text{FS}} \epsilon_{\mathbf{k}}. \quad (358)$$

Then we can determine from $1 = n_{\text{in}} + n_{\text{out}}$ and $g_t = n_{\text{in}} - n_{\text{out}}$ the densities

$$n_{\text{in}} = \frac{1 + g_t}{2}, \quad n_{\text{out}} = \frac{1 - g_t}{2}. \quad (359)$$

We thus find that there is a step in the distribution function (i.e., a quasiparticle picture makes sense), as long as $U < U_c$. Without derivation, we give two Fermi liquid parameters of the model

$$F_0^{\text{a}} = -\frac{U\nu(\epsilon_{\text{F}})}{4} \frac{2U_c + U}{(U + U_c)^2} U_c, \quad F_0^{\text{s}} = \frac{U\nu(\epsilon_{\text{F}})}{4} \frac{2U_c - U}{(U - U_c)^2} U_c. \quad (360)$$

One interesting feature about them is the divergence of F_0^{s} as $U \rightarrow U_c$. We recall that F_0^{s} appears in the denominator of the compressibility

$$\chi = \frac{\mu_{\text{B}}^2 \nu^*(\epsilon_{\text{F}})}{1 + F_0^{\text{a}}}, \quad \kappa = \frac{\nu^*(\epsilon_{\text{F}})}{n^2(1 + F_0^{\text{s}})}. \quad (361)$$

The renormalized density of states at the Fermi level $\nu^*(\epsilon_{\text{F}}) = m^* k_{\text{F}} / \pi^2$ diverges due to the diverging renormalized mass $m^* = m/g_t \propto (U - U_c)^{-1}$. However, the divergence in F_0^{s} is stronger so that, as expected for an insulator, the compressibility tends to zero. The spin susceptibility does diverge at the metal-insulator transition, due to the formation of completely independent local spins.

V. MAGNETISM IN SOLIDS

A. Antiferromagnetism

1. Superexchange in the Hubbard model

As discussed in the previous chapter, the Hubbard model has an extensive ground state degeneracy in the limit $t = 0$. We now study how this degeneracy is lifted when a small kinetic term $t \ll U$ is present. In order to derive an effective Hamiltonian, we consider the hopping process between two neighboring sites in second order perturbation theory (to get back to a ground state configuration, two hopping processes need to be involved). The two neighboring sites have four degenerate ground state configurations $|\uparrow, \uparrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\downarrow, \downarrow\rangle$. Acting with the kinetic part of the Hamiltonian on each of them yields

$$\begin{aligned} \hat{H}_{\text{kin}} |\uparrow, \uparrow\rangle &= \hat{H}_{\text{kin}} |\downarrow, \downarrow\rangle = 0, \\ \hat{H}_{\text{kin}} |\uparrow, \downarrow\rangle &= -\hat{H}_{\text{kin}} |\downarrow, \uparrow\rangle = -t|\uparrow\downarrow, 0\rangle - t|0, \uparrow\downarrow\rangle, \end{aligned} \quad (362)$$

where the relative minus sign in the last line is required by choosing a consistent ordering of the second quantized operators.

This way we obtain the matrix elements

$$M_{\sigma_1, \sigma_2; \sigma'_1, \sigma'_2} = - \frac{\langle \sigma_1, \sigma_2 | \hat{H}_{\text{kin}} | \uparrow \downarrow, 0 \rangle \langle \uparrow \downarrow, 0 | \hat{H}_{\text{kin}} | \sigma'_1, \sigma'_2 \rangle}{\langle \uparrow \downarrow, 0 | \hat{H}_U | \uparrow \downarrow, 0 \rangle} - \frac{\langle \sigma_1, \sigma_2 | \hat{H}_{\text{kin}} | 0, \uparrow \downarrow \rangle \langle 0, \uparrow \downarrow | \hat{H}_{\text{kin}} | \sigma'_1, \sigma'_2 \rangle}{\langle 0, \uparrow \downarrow | \hat{H}_U | 0, \uparrow \downarrow \rangle}, \quad (363)$$

where \hat{H}_U is the interaction part of the Hamiltonian. The denominator is U . The only nonzero matrix elements are allocated in the block

$$\begin{pmatrix} M_{\uparrow, \downarrow; \uparrow, \downarrow} & M_{\uparrow, \downarrow; \downarrow, \uparrow} \\ M_{\downarrow, \uparrow; \uparrow, \downarrow} & M_{\downarrow, \uparrow; \downarrow, \uparrow} \end{pmatrix} = -2t^2/U \begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix}. \quad (364)$$

which has the eigensystem

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad E = 0; \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad E = -\frac{4t^2}{U}. \quad (365)$$

The states $|\uparrow, \uparrow\rangle$ and $|\downarrow, \downarrow\rangle$ are two more eigenstates with zero energy. Together, the zero-energy states for a degenerate triplet, as required by the SU(2) spin-rotation symmetry of the Hamiltonian. The triplet $|\uparrow, \uparrow\rangle, (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)/\sqrt{2}, |\downarrow, \downarrow\rangle$ furnishes the eigenspace with eigenvalue $S(S+1)$ for $S = 1$ of the operator $(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2$. The singlet state $(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)/\sqrt{2}$ corresponds to the $S = 0$ eigenvalue. Using that

$$\begin{aligned} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2 &= \hat{\mathbf{S}}_1^2 + \hat{\mathbf{S}}_2^2 + 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \\ &= \frac{3}{4} + \frac{3}{4} + 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \end{aligned} \quad (366)$$

we can thus recast the effective Hamiltonian as

$$\hat{H}_{\text{eff};1-2} = J \left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4} \right), \quad J = \frac{4t^2}{U} > 0. \quad (367)$$

This spin-spin coupling mediated by a pair of virtual hopping processes, that we derived using second-order perturbation theory goes back to P.W. Anderson and is called *superexchange*. It can be used to derive this coupling between any two nearest-neighbor sites in the Hubbard model, yielding up to constant the effective Heisenberg Hamiltonian with antiferromagnetic coupling

$$\hat{H}_H = J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j. \quad (368)$$

As mentioned above, the model has a global $SU(2)$ spin rotation symmetry, represented by

$$R_{\alpha} = \exp \left[-i\alpha \cdot \sum_i \hat{S}_i \right]. \quad (369)$$

2. Mean-field theory and its shortcomings

We will now explore the ground state of the antiferromagnetic Heisenberg Hamiltonian (368). Surprisingly, there is a fundamental difference between the antiferromagnetic and the ferromagnetic Heisenberg model, even though they are related by just a global sign change in the Hamiltonian. The ferromagnetic problem is essentially classical: the ground state is of the form $|\uparrow\uparrow \cdots \uparrow\rangle$, we can compute its energy exactly. For the antiferromagnet, this is not true. The ground state deviates from $|\uparrow\downarrow \cdots \uparrow\downarrow\rangle$. The reason for this striking difference lies in the fact that the order parameter commutes with the Hamiltonian in the ferromagnetic case, while it does not commute in the antiferromagnet. If the order parameter commutes with the Hamiltonian, both have common eigenstates, and the ground state (necessarily an eigenstate of the Hamiltonian) can saturate the order parameter, as is uniquely realized by the $|\uparrow\uparrow \cdots \uparrow\rangle$ state in the ferromagnetic case. For the antiferromagnet, by the lack of commutation such a ideal ground state cannot be found. We say *quantum fluctuations* reduce the order parameter from the fully saturated value – the problem is intrinsically quantum-mechanical.

Let us be a bit more explicit about the (missing) commutation and the order parameters. The Heisenberg model is defined on a bipartite lattice, i.e., we can group the lattice sites in two sublattices A and B with a checkerboard arrangement, such that each site in A has only nearest neighbors in B and vice versa. The order parameters for ferro and antiferromagnet are then defined as

$$\begin{aligned} \hat{M}_{\text{fm}} &= \sum_{i \in A} \hat{S}_i + \sum_{j \in B} \hat{S}_j, \\ \hat{M}_{\text{afm}} &= \sum_{i \in A} \hat{S}_i - \sum_{j \in B} \hat{S}_j \end{aligned} \quad (370)$$

The lack of commutation can be seen from (for nearest neighbors $i \in A$ and $j \in B$)

$$\begin{aligned} [\hat{S}_{x,i} \hat{S}_{x,j} + \hat{S}_{y,i} \hat{S}_{y,j}, \hat{S}_{z,i}] &= i\hat{S}_{y,i} \hat{S}_{x,j} - i\hat{S}_{x,i} \hat{S}_{y,j}, \\ [\hat{S}_{x,i} \hat{S}_{x,j} + \hat{S}_{y,i} \hat{S}_{y,j}, \hat{S}_{z,j}] &= i\hat{S}_{x,i} \hat{S}_{y,j} - i\hat{S}_{y,i} \hat{S}_{x,j}. \end{aligned} \quad (371)$$

If the two terms are summed up as in $\widehat{\mathbf{M}}_{\text{fm}}$, the right-hand sides cancel, if we take their differences, as in $\widehat{\mathbf{M}}_{\text{afm}}$, they don't.

While the symmetry is spontaneously broken in the antiferromagnetic ground state $\langle \widehat{\mathbf{M}}_{\text{afm}} \rangle \neq 0$, mean-field theory is not going to deliver the exact ground state. Nevertheless, it is instructive to perform a mean-field calculation for the problem. We write

$$\begin{aligned}\hat{\mathbf{S}}_i &= M\hat{\mathbf{e}}_z + (\hat{\mathbf{S}}_i - M\hat{\mathbf{e}}_z), & i \in \text{A} \\ \hat{\mathbf{S}}_j &= -M\hat{\mathbf{e}}_z + (\hat{\mathbf{S}}_j + M\hat{\mathbf{e}}_z), & j \in \text{B}\end{aligned}\tag{372}$$

introducing the mean field M . The effective Hamiltonian is

$$\hat{H}_{\text{mf}} = -JzM \sum_{i \in \text{A}} \hat{S}_{z,i} + JzM \sum_{i \in \text{A}} \hat{S}_{z,i} + J\frac{z}{2}M^2N,\tag{373}$$

where we returned to a general case of coordination number z . The partition function

$$\begin{aligned}Z_N(\beta, M) &= \text{tr} e^{\beta \hat{H}_{\text{mf}}} \\ &= e^{-\beta J\frac{z}{2}M^2N} \left(e^{\beta JMz/2} + e^{-\beta JMz/2} \right)^N\end{aligned}\tag{374}$$

is *identical* to the ferromagnetic case of Eq. (45), which shows again that the mean-field theory is not capable of detecting the differences between antiferromagnetic and ferromagnetic order. There follows the identical transition temperature, which for the antiferromagnet is called Neel temperature

$$T_{\text{N}} = \frac{Jz}{4k_{\text{B}}}.\tag{375}$$

Clearly, the larger the coupling constant J and the more neighbors are present, the more stable is the ordered state. Close to the transition, we can expand the free energy in M

$$F(M, T) = F_0 + \frac{Jz}{2} \left[\left(1 - \frac{T_{\text{N}}}{T} \right) M^2 + \frac{2}{3} \left(\frac{T_{\text{N}}}{T} \right)^3 M^4 \right].\tag{376}$$

This effective free energy describes a second-order phase transition. Minimization of F with respect to M yields the characteristic mean-field temperature dependence of the order parameter

$$M(T) = \frac{1}{2} \frac{T}{T_{\text{N}}} \sqrt{3 \left(1 - \frac{T}{T_{\text{N}}} \right)}, \quad T \leq T_{\text{N}},\tag{377}$$

while $M(T)$ vanishes for $T > T_{\text{N}}$.

3. Spin-wave theory

We are going to study spin-wave excitations (magnons) on top of the ferromagnetically and antiferromagnetically ordered state. We will treat this problem using the so-called Holstein-Primakoff transformation, which allows to rewrite the spin operators at each lattice site in terms of creation and annihilation operators of a boson. The virtue of this transformation is that the algebra of bosons is much simpler than that of spins. However, the price to pay is that the bosonic operators are acting on a larger local Hilbert space at every lattice site than the spin operators. In this way, one might end up with solutions of the bosonic problem, that do not map back to physical states in the spin variables. This problem is avoided in the approximation by which spins only deviate slightly from the ferromagnetic or antiferromagnetic orientation, as we shall see below.

Our goal is to derive the dispersion relations of spin waves and to understand their connections to the symmetries of the problem. For small momenta \mathbf{k} , the dispersions will be quadratic in \mathbf{k} in the ferromagnet and linear in \mathbf{k} in the antiferromagnet. We will discuss the general spin- S case and particularize on the spin-1/2 model discussed so far in the end. On every lattice site i , the components $\hat{S}_{i,\alpha}$ with $\alpha = x, y, z$ of the spin operator act on the $(2S + 1)$ -dimensional local Hilbert space

$$\mathcal{H}_i^s = \text{span}\{|-S\rangle_i, |-S+1\rangle_i, \dots, |S-1\rangle_i, |S\rangle_i\}, \quad (378)$$

which we have chosen to represent with the eigenbasis of $\hat{S}_{i,z}$,

$$\hat{S}_{i,z}|m\rangle_i = m|m\rangle_i, \quad m = -S, -S+1, \dots, S-1, S. \quad (379)$$

In order to perform the Holstein-Primakoff transformation, we consider introducing a bosonic degree of freedom at every lattice site i with creation and annihilation operators \hat{a}_i^\dagger and \hat{a}_i , respectively, that act on the local infinite-dimensional Hilbert space

$$\mathcal{H}_i^b = \text{span}\left\{|n\rangle_i := (n!)^{-1/2} \hat{a}_i^{\dagger n} |0\rangle_i \mid n = 0, 1, 2, \dots; \hat{a}_i |0\rangle_i = 0\right\}, \quad (380)$$

and obey

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j}, \quad (381)$$

with all other commutators vanishing.

a. Ferromagnetic case The Holstein-Primakoff transformation is defined by introducing the following substitutes for the spin operators

$$\widehat{\mathcal{S}}_i^+ := \sqrt{2S - \widehat{a}_i^\dagger \widehat{a}_i} \widehat{a}_i, \quad \widehat{\mathcal{S}}_i^- := \widehat{a}_i^\dagger \sqrt{2S - \widehat{a}_i^\dagger \widehat{a}_i}, \quad \widehat{\mathcal{S}}_i^z := S - \widehat{a}_i^\dagger \widehat{a}_i. \quad (382)$$

One verifies that these spin wave operators obey the same algebra

$$[\widehat{\mathcal{S}}_i^+, \widehat{\mathcal{S}}_i^-] = 2\widehat{\mathcal{S}}_i^z, \quad [\widehat{\mathcal{S}}_i^\pm, \widehat{\mathcal{S}}_i^z] = \mp \widehat{\mathcal{S}}_i^\pm \quad (383)$$

on \mathcal{H}_i^b as the original spin operators do on \mathcal{H}_i^s (where $\widehat{S}_i^\pm := \widehat{S}_{i,x} \pm i\widehat{S}_{i,y}$). Now, the central assumption that will allow us to simplify the theory when written in the bosonic variables is that the fraction of reversed spins above the ferromagnetic ground state is small

$$\langle \widehat{a}_i^\dagger \widehat{a}_i \rangle / S \ll 1, \quad \forall i. \quad (384)$$

Within the range of validity of this assumption, it is justified to expand the square-roots that enter Eq. (382) in $\widehat{a}_i^\dagger \widehat{a}_i / (2S)$. Of course, this will be better justified, the larger S is, i.e., the more “classical” the spin behaves.

It is furthermore useful to introduce the Fourier transforms of the bosonic operators

$$\widehat{c}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{r}_i \cdot \mathbf{k}} \widehat{a}_i^\dagger, \quad \widehat{c}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{r}_i \cdot \mathbf{k}} \widehat{a}_i. \quad (385)$$

Using these together with Eq. (382), and expanding the square root to lowest order, the Hamiltonian

$$\widehat{H}_{\text{fm}} = -J \sum_{\langle i,j \rangle} \widehat{\mathbf{S}}_i \cdot \widehat{\mathbf{S}}_j - B \sum_i \widehat{S}_{i,z} \quad (386)$$

becomes

$$\widehat{H}'_{\text{fm}} = -JN \frac{z}{2} S^2 - BNS - JzS \sum_{\mathbf{k}} \left(\frac{\gamma_{\mathbf{k}} + \gamma_{-\mathbf{k}}}{2} - 1 \right) \widehat{c}_{\mathbf{k}}^\dagger \widehat{c}_{\mathbf{k}} + B \sum_{\mathbf{k}} \widehat{c}_{\mathbf{k}}^\dagger \widehat{c}_{\mathbf{k}} \quad (387)$$

where

$$\gamma_{\mathbf{k}} = \frac{2}{z} \sum_{\boldsymbol{\delta}} e^{i\mathbf{k} \cdot \boldsymbol{\delta}}, \quad (388)$$

$\boldsymbol{\delta}$ are the *directed* connection vectors to nearest neighbors and z is the coordination number.

Using $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}^*$ and dropping the constant terms in this Hamiltonian, we arrive at

$$\widehat{H}''_{\text{fm}} = \sum_{\mathbf{k}} [JzS(1 - \text{Re}\gamma_{\mathbf{k}}) + B] \widehat{c}_{\mathbf{k}}^\dagger \widehat{c}_{\mathbf{k}}. \quad (389)$$

From this we can directly read off the dispersion of the ferromagnetic magnons as

$$\begin{aligned}\omega_{\mathbf{k}} &= JzS(1 - \text{Re}\gamma_{\mathbf{k}}) + B \\ &\approx B + JSa^2\mathbf{k}^2,\end{aligned}\tag{390}$$

where we assumed a hypercubic lattice with lattice constant a to obtain the last line. This is equivalent to the dispersion of a free massive particle with mass $m^* = 1/(2JSa^2)$.

b. Antiferromagnetic case For the antiferromagnetic case, we have to account for the two sublattices when performing the Holstein-Primakov transformation and we have to replace the source field B by a staggered one. We are thus interested in the Hamiltonian

$$\hat{H}_{\text{afm}} = J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - B \sum_{i \in A} \hat{S}_{i,z} + B \sum_{j \in B} \hat{S}_{j,z},\tag{391}$$

and introduce on sublattice A the operators

$$\hat{\mathcal{S}}_i^+ := \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i} \hat{a}_i, \quad \hat{\mathcal{S}}_i^- := \hat{a}_i^\dagger \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i}, \quad \hat{\mathcal{S}}_i^z := S - \hat{a}_i^\dagger \hat{a}_i.\tag{392}$$

while on sublattice B we use the operators

$$\hat{\mathcal{S}}_j^+ := \hat{b}_j^\dagger \sqrt{2S - \hat{b}_j^\dagger \hat{b}_j}, \quad \hat{\mathcal{S}}_j^- := \sqrt{2S - \hat{b}_j^\dagger \hat{b}_j} \hat{b}_j, \quad \hat{\mathcal{S}}_j^z := \hat{b}_j^\dagger \hat{b}_j - S.\tag{393}$$

Both the \hat{a}_j^\dagger and \hat{b}_j^\dagger obey the usual bosonic algebra. It is again convenient to introduce Fourier transforms of these bosonic operators

$$\begin{aligned}\hat{c}_{\mathbf{k}}^\dagger &= \frac{1}{\sqrt{N_A}} \sum_{i \in A} e^{-i\mathbf{r}_i \cdot \mathbf{k}} \hat{a}_i^\dagger, & \hat{c}_{\mathbf{k}} &= \frac{1}{\sqrt{N_A}} \sum_{i \in A} e^{i\mathbf{r}_i \cdot \mathbf{k}} \hat{a}_i, \\ \hat{d}_{\mathbf{k}}^\dagger &= \frac{1}{\sqrt{N_B}} \sum_{j \in B} e^{-i\mathbf{r}_j \cdot \mathbf{k}} \hat{b}_j^\dagger, & \hat{d}_{\mathbf{k}} &= \frac{1}{\sqrt{N_B}} \sum_{j \in B} e^{i\mathbf{r}_j \cdot \mathbf{k}} \hat{b}_j,\end{aligned}\tag{394}$$

where $N_A = N_B = N/2$. Furthermore allowing for a linear transformation

$$\hat{\alpha}_{\mathbf{k}} = u_{\mathbf{k}} \hat{c}_{\mathbf{k}} - v_{\mathbf{k}} \hat{d}_{\mathbf{k}}^\dagger, \quad \hat{\beta}_{\mathbf{k}} = u_{\mathbf{k}} \hat{d}_{\mathbf{k}} - v_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger,\tag{395}$$

with $1 = u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2$, which ensures $[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}}^\dagger] = [\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}^\dagger] = 1$, we can cast the Hamiltonian (391), expanding in the bosonic operators, in the form

$$\hat{H}'_{\text{afm}} = -JN \frac{z}{2} S(S+1) - \frac{1}{2} BN(2S+1) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} + 1 \right).\tag{396}$$

The antiferromagnetic magnon dispersion is given by

$$\begin{aligned}\omega_{\mathbf{k}} &= \sqrt{(JzS + B)^2 - (JzS \operatorname{Re} \gamma_{\mathbf{k}})^2} \\ &\approx 2\sqrt{3}JS\mathbf{a}|\mathbf{k}|,\end{aligned}\tag{397}$$

where we have expanded in small momenta $\mathbf{a}|\mathbf{k}| \ll 1$ for the case of a hypercubic lattice for $B = 0$ in the last line. Notice that in contrast to the ferromagnetic case, this is a gapless dispersion.

This sharp difference between the ferro- and antiferromagnetic case is rooted in the property that the order parameter commutes and does not commute with the Hamiltonian in the two cases, respectively.

We can expand on this observation by considering the symmetries of Hamiltonians (386) and (391) in the limit $B = 0$. The Hamiltonians, if the lattice Λ has the space group \mathcal{P}_Λ as symmetry group, has the symmetry group

$$G_\Lambda = \operatorname{SO}(3) \times \mathbb{Z}_2 \times \mathcal{P}_\Lambda,\tag{398}$$

where $\operatorname{SO}(3)$ are the proper rotations in spin space and \mathbb{Z}_2 is time-reversal. For the antiferromagnetic order, we anticipate a reduction of the point group symmetry to \mathcal{P}_{Λ_A} of the A sublattice only, where $\mathcal{P}_\Lambda = \mathbb{Z}_2 \times \mathcal{P}_{\Lambda_A}$. Notice that all symmetries but time reversal are unitary here.

For the ferromagnet, the order parameter \widehat{M} is actually one of the generators of the continuous global symmetry group $\operatorname{SO}(3)$. This is the reason why it commutes with the Hamiltonian. When acquiring a nonzero expectation value, \widehat{M} breaks $\operatorname{SO}(3)$ down to $\operatorname{SO}(2)$ (rotations around the ferromagnetic axis) and at the same time breaks time-reversal symmetry. The symmetry-breaking pattern is thus

$$G_\Lambda = \operatorname{SO}(3) \times \mathbb{Z}_2 \times \mathcal{P}_\Lambda \longrightarrow H_{\Lambda,\text{fm}} = \operatorname{SO}(2) \times \mathcal{P}_\Lambda.\tag{399}$$

For the antiferromagnet, the order parameter similarly breaks $\operatorname{SO}(3)$ down to $\operatorname{SO}(2)$ and breaks time-reversal. It does, however, preserve an ‘effective time-reversal symmetry’, that is a composition of time-reversal symmetry and a translation that interchanges the sublattices A and B. This yields the symmetry breaking pattern

$$G_\Lambda = \operatorname{SO}(3) \times \mathbb{Z}_2 \times \mathcal{P}_\Lambda \longrightarrow H_{\Lambda,\text{afm}} = \operatorname{SO}(2) \times \mathbb{Z}_2 \times \mathcal{P}_{\Lambda_A}.\tag{400}$$

The fundamental difference between $H_{\Lambda,\text{fm}}$ and $H_{\Lambda,\text{afm}}$ is that the latter still contains an antiunitary symmetry (the effective time reversal symmetry).

As stated before, the ferromagnetic ground state coincides with the quantum-mechanical one, but this is not true for the antiferromagnet. To quantify this we compute the deviation ΔM of the fully polarized classical sublattice magnetization $NS/2$ with the quantum mechanical one within the approximation (384), i.e.,

$$\Delta M = \frac{NS}{2} - \left\langle \sum_{i \in \Lambda} \hat{\mathcal{S}}_{i,z} \right\rangle, \quad (401)$$

where the brackets stand for the ground state expectation value. With the form of Hamiltonian (396) this quantity can be computed as

$$\begin{aligned} \Delta M &= \frac{1}{2} \sum_{\mathbf{k}} \left(\frac{1}{\sqrt{1 - (\text{Re}\gamma_{\mathbf{k}})^2}} - 1 \right) \\ &= -\frac{N}{4} + \frac{1}{2(2\pi)^3} \int d^3\mathbf{k} \frac{1}{\sqrt{1 - (\text{Re}\gamma_{\mathbf{k}})^2}} \\ &\approx 0.0784 \frac{N}{2}, \end{aligned} \quad (402)$$

meaning that we obtain a nearly 8 percent reduction from the fully polarized magnetization.

B. Stoner magnetism

In this section we are going to explore magnetism from a different angle, namely starting from itinerant electrons. Magnetism arises here as an instability of a Fermi liquid, without the need for a picture of localized moments and thus without the underlying lattice playing an important role. Examples of magnets for which this mechanism is at work include the ferromagnets iron, cobalt, and nickel, in all of which $3d$ -orbital electrons dominate the states at the Fermi energy. The ferromagnetic order is a spontaneous symmetry breaking phenomenon appearing at some finite T_c , the Curie temperature. The phase transition is of second order in the Landau classification of phase transitions, thus featuring a discontinuity in the specific heat but none in the entropy and volume.

Stoner magnetism is driven by repulsive (Coulomb) interactions. The energy gain can be understood from Hund's rule: Alignment of the electronic spins in a favored direction allows them to reduce the Coulomb energy. We recall that within Fermi liquid theory we have

found

$$\chi = \frac{m^*}{m} \frac{\chi_0}{1 + F_0^a}, \quad (403)$$

for the magnetic susceptibility and concluded that a ferromagnetic instability would occur if $F_0^a \rightarrow -1$. We will now use mean-field theory to derive this more microscopically.

1. Mean-field theory

We start from the Hamiltonian with a repulsive contact interaction

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} + U \int d^3 \mathbf{r} d^3 \mathbf{r}' \hat{\rho}_\uparrow(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \hat{\rho}_\downarrow(\mathbf{r}'), \quad (404)$$

where $\hat{\rho}_\sigma(\mathbf{r}) = \hat{\phi}_\sigma^\dagger(\mathbf{r}) \hat{\phi}_\sigma(\mathbf{r})$ is the density operator with $\hat{\phi}_\sigma^\dagger(\mathbf{r})$ the electron field operators. We use this contact interaction as a simple model for screened Coulomb interaction. It is clear that electrons of the same spin are not affected by the interaction, which gives rise to the Hund's rule mentioned above. We make the mean-field ansatz

$$\hat{\rho}_\sigma(\mathbf{r}) = \bar{n}_\sigma + [\hat{\rho}_\sigma(\mathbf{r}) - \bar{n}_\sigma], \quad (405)$$

with $\bar{n}_\sigma = \langle \hat{\rho}_\sigma(\mathbf{r}) \rangle$ and the brackets represent the thermal average. To justify a mean-field Hamiltonian, we assume

$$\langle [\hat{\rho}_\downarrow(\mathbf{r}) - \bar{n}_\downarrow] [\hat{\rho}_\uparrow(\mathbf{r}) - \bar{n}_\uparrow] \rangle \ll \bar{n}_\downarrow \bar{n}_\uparrow. \quad (406)$$

Then

$$\begin{aligned} \hat{H}_{\text{mf}} &= \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} + U \int d^3 \mathbf{r} [\hat{\rho}_\uparrow(\mathbf{r}) \bar{n}_\downarrow + \hat{\rho}_\downarrow(\mathbf{r}) \bar{n}_\uparrow - \bar{n}_\downarrow \bar{n}_\uparrow] \\ &= \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} + U \bar{n}_{-\sigma}) \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} - \Omega U \bar{n}_\downarrow \bar{n}_\uparrow. \end{aligned} \quad (407)$$

This mean-field Hamiltonian describes electrons of one spin type σ moving in the background of the opposite spin electrons $-\sigma$. We thus reduced the problem again to a single-particle like problem. This is at the heart of the so-called Hartree-Fock approximation. To find a

self-consistent solution, we calculate the spin density

$$\begin{aligned}
\bar{n}_\uparrow &= \frac{1}{\Omega} \sum_{\mathbf{k}} \langle \hat{c}_{\mathbf{k},\uparrow}^\dagger \hat{c}_{\mathbf{k},\uparrow} \rangle \\
&= \frac{1}{\Omega} \sum_{\mathbf{k}} n_{\epsilon_{\mathbf{k}} + U\bar{n}_\downarrow} \\
&= \int d\epsilon \frac{1}{\Omega} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}} - U\bar{n}_\downarrow) n_\epsilon \\
&= \int d\epsilon \frac{1}{2} \nu(\epsilon - U\bar{n}_\downarrow) n_\epsilon,
\end{aligned} \tag{408}$$

where n_ϵ is the Fermi Dirac distribution. The analogous equation holds for \bar{n}_\downarrow . These equations allow to self-consistently determine the mean densities \bar{n}_σ . Solutions must obey particle number conservation. To implement this, it is convenient to split up the spin densities in average particle densities \bar{n} and magnetization \bar{m} , the latter being related to the measurable magnetization density $M = \mu_B \bar{m}$. That is

$$\bar{n}_\sigma = \frac{\bar{n} + \sigma \bar{m}}{2}. \tag{409}$$

The self-consistency equations can then be cast in the form

$$\begin{aligned}
\bar{n} &= \frac{1}{2} \int d\epsilon [\nu(\epsilon - U\bar{n}_\downarrow) + \nu(\epsilon - U\bar{n}_\uparrow)] n_\epsilon \\
\bar{m} &= \frac{1}{2} \int d\epsilon [\nu(\epsilon - U\bar{n}_\downarrow) - \nu(\epsilon - U\bar{n}_\uparrow)] n_\epsilon
\end{aligned} \tag{410}$$

or

$$\begin{aligned}
\bar{n} &= \frac{1}{2} \int d\epsilon \sum_{\sigma} \nu(\epsilon - U\bar{n}/2 - \sigma U\bar{m}/2) n_\epsilon \\
\bar{m} &= \frac{1}{2} \int d\epsilon \sum_{\sigma} \sigma \nu(\epsilon - U\bar{n}/2 - \sigma U\bar{m}/2) n_\epsilon.
\end{aligned} \tag{411}$$

To make analytical progress from here, we assume that the magnetization is small, i.e., $\bar{m} \ll \bar{n}$. We absorb the shift $-U\bar{n}/2$ in the Fermi energy and expand (for the case of \bar{n} , where the \bar{m} -odd term vanishes by the sum over σ)

$$\nu(\epsilon - \sigma U\bar{m}/2) = \nu(\epsilon) + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \nu''(\epsilon) + \mathcal{O}(m^4). \tag{412}$$

We furthermore use the so-called Sommerfeld expansion

$$\int_{-\infty}^{\infty} h(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon = \int_{-\infty}^{\mu} h(\epsilon) d\epsilon + \frac{\pi^2}{6\beta^2} h'(\mu) + \mathcal{O}(\beta\mu)^{-4}. \tag{413}$$

Lastly, we have to allow for a \bar{m} -dependent shift in the chemical potential, i.e., $\mu(\bar{m}, T) = \epsilon_F + \delta\mu(\bar{m}, T)$, such that $\delta\mu(0, T) = 0$. Together, when expanded to lowest order both in m and in β^{-1} , this yields

$$\begin{aligned}\bar{n} &= \int_{-\infty}^{\mu} d\epsilon \nu(\epsilon) + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \nu'(\epsilon_F) + \frac{\pi^2}{6\beta^2} \nu'(\epsilon_F) \\ &= \int_{-\infty}^{\epsilon_F} d\epsilon \nu(\epsilon) + \delta\mu \nu(\epsilon_F) + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \nu'(\epsilon_F) + \frac{\pi^2}{6\beta^2} \nu'(\epsilon_F) \\ &= \bar{n} + \delta\mu \nu(\epsilon_F) + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \nu'(\epsilon_F) + \frac{\pi^2}{6\beta^2} \nu'(\epsilon_F).\end{aligned}\tag{414}$$

We can now solve for $\delta\mu$ as

$$\delta\mu(\bar{m}, T) = -\frac{\nu'(\epsilon_F)}{\nu(\epsilon_F)} \left[\frac{\pi^2}{6\beta^2} + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \right].\tag{415}$$

The analogous calculation for \bar{m} reads

$$\begin{aligned}\bar{m} &= \int d\epsilon n_{\epsilon} \left[\nu'(\epsilon) \frac{U\bar{m}}{2} + \frac{1}{3!} \nu'''(\epsilon) \left(\frac{U\bar{m}}{2} \right)^3 \right] \\ &= \frac{U\bar{m}}{2} \left[\nu(\epsilon_F) + \delta\mu \nu'(\epsilon_F) + \frac{\pi^2}{6\beta^2} \nu''(\epsilon_F) + \frac{1}{3!} \left(\frac{U\bar{m}}{2} \right)^2 \nu''(\epsilon_F) \right] \\ &= \frac{U\bar{m}}{2} \nu \left[1 - \frac{\nu'^2}{\nu^2} \left[\frac{\pi^2}{6\beta^2} + \frac{1}{2} \left(\frac{U\bar{m}}{2} \right)^2 \right] + \frac{\pi^2}{6\beta^2} \frac{\nu''}{\nu} + \frac{1}{3!} \left(\frac{U\bar{m}}{2} \right)^2 \frac{\nu''}{\nu} \right] \\ &= \nu \left[\frac{U\bar{m}}{2} \left(1 - \frac{\pi^2}{6\beta^2} \frac{\nu'^2}{\nu^2} + \frac{\pi^2}{6\beta^2} \frac{\nu''}{\nu} \right) + \left(\frac{U\bar{m}}{2} \right)^3 \left(\frac{1}{3!} \frac{\nu''}{\nu} - \frac{1}{2} \frac{\nu'^2}{\nu^2} \right) \right],\end{aligned}\tag{416}$$

where we dropped the ϵ_F argument in the last line for notational compactness and inserted $\delta\mu$ from Eq. (415).

The structure of this equation is $\bar{m} = a\bar{m} + b\bar{m}^3$. If b is negative, we have two possible solutions

$$\begin{aligned}\bar{m} &= 0, & a < 1, \\ \bar{m} &= \frac{1-a}{b}, & a \geq 1.\end{aligned}\tag{417}$$

Obviously, the second solution is the one in the symmetry broken phase and hence $a = 1$ the critical value. Via the temperature dependence of a we can determine the critical temperature (the Curie temperature)

$$1 = \frac{U\nu}{2} \left[1 - \frac{\pi^2}{6\beta^2} \left(\frac{\nu'^2}{\nu^2} - \frac{\nu''}{\nu} \right) \right]\tag{418}$$

yielding

$$k_{\text{B}}T_{\text{c}} = \frac{\sqrt{6}}{\pi \sqrt{\frac{\nu'^2}{\nu^2} - \frac{\nu''}{\nu}}} \sqrt{1 - \frac{2}{U\nu}} \propto \sqrt{1 - \frac{U_{\text{c}}}{U}}, \quad (419)$$

for $U > U_{\text{c}} = 2/\nu(\epsilon_{\text{F}})$. The latter condition

$$U\nu(\epsilon_{\text{F}}) > 2 \quad (420)$$

on the minimal interaction strength is the instability condition for the paramagnetic Fermi liquid to turn ferromagnetic at low temperatures, called the *Stoner condition*. For $U\nu(\epsilon_{\text{F}}) < 2$ there is no phase transition. In the symmetry-breaking phase ($T < T_{\text{c}}$), the magnetization has the characteristic mean-field temperature-dependence

$$\bar{m}(T) \propto \sqrt{T_{\text{c}} - T}. \quad (421)$$

This dependence is valid sufficiently close to the transition $T - T_{\text{c}} \ll T_{\text{c}}$. Since the density of states can also be changed by applying pressure, say, the phase transition can also be driven a zero temperature if system parameters are changed such that the $U\nu(\epsilon_{\text{F}}) = 2$ is crossed. A phase transition at zero temperature is called a *quantum phase transition*.

2. Susceptibility on the paramagnetic side

To compute the susceptibility, we apply a small symmetry-breaking field B along the spin-quantization direction by adding the following Zeeman term to the Hamiltonian (407) (setting the g -factor equal to 2)

$$\hat{H}_{\text{Z}} = -\mu_{\text{B}} \int d^3\mathbf{r} B [\hat{\rho}_{\uparrow}(\mathbf{r}) - \hat{\rho}_{\downarrow}(\mathbf{r})]. \quad (422)$$

The self-consistency equations (416) are now modified by replacing $U\bar{m}/2$ with $U\bar{m}/2 + \mu_{\text{B}}B$ on the right-hand side. We only keep the \bar{m} -linear terms this time

$$\bar{m} = \nu \left(\frac{U\bar{m}}{2} + \mu_{\text{B}}B \right) \left(1 - \frac{\pi^2}{6\beta^2} \frac{\nu'^2}{\nu^2} + \frac{\pi^2}{6\beta^2} \frac{\nu''}{\nu} \right) \quad (423)$$

We can solve this equation for \bar{m} and then compute the susceptibility χ via $\chi = M/B$ with $M = \mu_{\text{B}}\bar{m}$. The result is given by

$$\chi(T) = \frac{M}{B} = \frac{\chi_0(T)}{1 - \frac{U\chi_0(T)}{2\mu_{\text{B}}^2}}, \quad (424)$$

where

$$\chi_0(T) = \mu_B^2 \nu \left[1 - \frac{\pi^2}{6\beta^2} \left(\frac{\nu'^2}{\nu^2} - \frac{\nu''}{\nu} \right) \right]. \quad (425)$$

Notice that the denominator of $\chi(T)$ vanishes exactly when Eq. (418) is satisfied, i.e., at the phase transition at finite temperature. From the paramagnetic side, the susceptibility diverges as

$$\chi(T) \approx \frac{\chi_0(T_c)}{\frac{T_c^2}{T^2} - 1} \propto |T - T_c|^{-1}, \quad (426)$$

which is the characteristic mean-field behavior with critical exponent 1. Notice also, that in passing we have determined the Landau parameter

$$F_0^a = -\frac{U\chi_0}{2\mu_B^2}, \quad (427)$$

which, as expected, is proportional to the interaction strength in the Fermi liquid.

3. Magnons

We have already encountered magnons as elementary excitations on top of the ferromagnetic ground state of the Heisenberg model using the spin-wave approximation. Here we study how magnons arise in the itinerant ferromagnet that has undergone a Stoner-instability. To that end, we consider particle-hole excitations with momentum \mathbf{q} by making the ansatz

$$|\Psi_{\mathbf{q}}\rangle = \sum_{\mathbf{k}} a_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{q},\downarrow}^\dagger \hat{c}_{\mathbf{k},\uparrow} |0\rangle, \quad (428)$$

where $|0\rangle$ is the (symmetry-broken) ground state and $a_{\mathbf{k}}$ are coefficients. To find potential eigenstates of this form, we solve the Schrödinger equation

$$\hat{H}|\Psi_{\mathbf{q}}\rangle = (E_0 + \omega_{\mathbf{q}})|\Psi_{\mathbf{q}}\rangle, \quad (429)$$

where $\hat{H}|0\rangle = E_0|0\rangle$. We can recast this as

$$\omega_{\mathbf{q}}|\Psi_{\mathbf{q}}\rangle = \sum_{\mathbf{k}} a_{\mathbf{k}} \left[\hat{H}, \hat{c}_{\mathbf{k}+\mathbf{q},\downarrow}^\dagger \hat{c}_{\mathbf{k},\uparrow} \right] |0\rangle \quad (430)$$

As before, we are going to employ a Hamiltonian with on-site interaction

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k},\sigma}^\dagger \hat{c}_{\mathbf{k},\sigma} + \frac{U}{\Omega} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{c}_{\mathbf{k}+\mathbf{q},\uparrow}^\dagger \hat{c}_{\mathbf{k},\uparrow} \hat{c}_{\mathbf{k}'-\mathbf{q},\downarrow}^\dagger \hat{c}_{\mathbf{k}',\downarrow}. \quad (431)$$

with the help of which we can compute the commutator (430) as

$$\omega_q |\Psi_q\rangle = (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) |\Psi_q\rangle + \frac{U}{\Omega} \sum_{\mathbf{k}} a_{\mathbf{k}} \sum_{\mathbf{k}', \mathbf{q}'} \left(\hat{c}_{\mathbf{k}'+\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}', \uparrow}^\dagger \hat{c}_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} - \hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}'-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}', \downarrow} \right) |0\rangle. \quad (432)$$

We now make an approximation by which we replace pairs of \hat{c} operators by their expectation values $n_{\mathbf{k}, \sigma}$ according to the Fermi-Dirac distribution

$$\begin{aligned} \hat{c}_{\mathbf{k}'+\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}', \uparrow}^\dagger \hat{c}_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} &\rightarrow \delta_{\mathbf{q}', 0} n_{\mathbf{k}', \uparrow} \hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} - \delta_{\mathbf{k}, \mathbf{k}'+\mathbf{q}'} n_{\mathbf{k}, \uparrow} \hat{c}_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}, \\ -\hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}'-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}', \downarrow} &\rightarrow -\delta_{\mathbf{q}', 0} n_{\mathbf{k}', \downarrow} \hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} + n_{\mathbf{k}+\mathbf{q}, \downarrow} \delta_{\mathbf{k}', \mathbf{k}+\mathbf{q}} \hat{c}_{\mathbf{k}-\mathbf{q}'+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}, \end{aligned} \quad (433)$$

which together give

$$\begin{aligned} &\hat{c}_{\mathbf{k}'+\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}', \uparrow}^\dagger \hat{c}_{\mathbf{k}+\mathbf{q}-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} - \hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}^\dagger \hat{c}_{\mathbf{k}'-\mathbf{q}', \downarrow}^\dagger \hat{c}_{\mathbf{k}', \downarrow} \\ &\rightarrow \delta_{\mathbf{q}', 0} (n_{\mathbf{k}', \uparrow} - n_{\mathbf{k}', \downarrow}) \hat{c}_{\mathbf{k}+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}, \uparrow} + (n_{\mathbf{k}+\mathbf{q}, \downarrow} \delta_{\mathbf{k}', \mathbf{k}+\mathbf{q}} - n_{\mathbf{k}, \uparrow} \delta_{\mathbf{k}, \mathbf{k}'+\mathbf{q}'}) \hat{c}_{\mathbf{k}-\mathbf{q}'+\mathbf{q}, \downarrow}^\dagger \hat{c}_{\mathbf{k}-\mathbf{q}', \uparrow}. \end{aligned} \quad (434)$$

This approximation yields an iteration of Eq. (432), that when projected on the state $\langle 0 | \hat{c}_{\tilde{\mathbf{k}} \uparrow}^\dagger \hat{c}_{\tilde{\mathbf{k}}+\mathbf{q} \downarrow}$ reads

$$a_{\tilde{\mathbf{k}}} [\omega_q - \epsilon_{\tilde{\mathbf{k}}+\mathbf{q}, \downarrow} + \epsilon_{\tilde{\mathbf{k}}, \uparrow}] = \frac{U}{\Omega} \sum_{\mathbf{k}} a_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{q}, \downarrow} - n_{\mathbf{k}, \uparrow}), \quad (435)$$

where we defined

$$\epsilon_{\mathbf{k}, \sigma} = \epsilon_{\mathbf{k}} + U n_{-\sigma} \quad (436)$$

in terms of the density of spin σ

$$n_{\sigma} = \frac{1}{\Omega} \sum_{\mathbf{k}'} n_{\mathbf{k}', \sigma}. \quad (437)$$

The goal is now to find the eigenvalues that solve Eq. (435) (we are not necessarily interested in the eigenstates $a_{\tilde{\mathbf{k}}}$. To that end, we rewrite Eq. (435) as

$$a_{\tilde{\mathbf{k}}} = \frac{U}{\Omega} \frac{1}{\omega_q - \epsilon_{\tilde{\mathbf{k}}+\mathbf{q}, \downarrow} + \epsilon_{\tilde{\mathbf{k}}, \uparrow}} \sum_{\mathbf{k}} a_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{q}, \downarrow} - n_{\mathbf{k}, \uparrow}), \quad (438)$$

multiply both sides by $n_{\tilde{\mathbf{k}}+\mathbf{q} \downarrow} - n_{\tilde{\mathbf{k}} \uparrow}$ and sum over $\tilde{\mathbf{k}}$

$$\left[\sum_{\tilde{\mathbf{k}}} a_{\tilde{\mathbf{k}}} (n_{\tilde{\mathbf{k}}+\mathbf{q} \downarrow} - n_{\tilde{\mathbf{k}} \uparrow}) \right] = \frac{U}{\Omega} \sum_{\tilde{\mathbf{k}}} \frac{n_{\tilde{\mathbf{k}}+\mathbf{q} \downarrow} - n_{\tilde{\mathbf{k}} \uparrow}}{\omega_q - \epsilon_{\tilde{\mathbf{k}}+\mathbf{q}, \downarrow} + \epsilon_{\tilde{\mathbf{k}}, \uparrow}} \left[\sum_{\mathbf{k}} a_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{q}, \downarrow} - n_{\mathbf{k}, \uparrow}) \right]. \quad (439)$$

The terms in square brackets cancel and we are left with

$$1 = \frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q} \downarrow} - n_{\mathbf{k} \uparrow}}{\omega_q - \epsilon_{\mathbf{k}+\mathbf{q}, \downarrow} + \epsilon_{\mathbf{k}, \uparrow}}. \quad (440)$$

This equation has solutions for $\omega_{\mathbf{q}} = \epsilon_{\mathbf{k}+\mathbf{q},\downarrow} - \epsilon_{\mathbf{k},\uparrow} = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + U(n_{\uparrow} - n_{\downarrow}) \equiv \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + \Delta$, which defines a particle-hole continuum at finite energy (for small \mathbf{q}). Setting $\mathbf{q} = 0$ we find in addition zero energy excitations because

$$1 = U \frac{n_{\downarrow} - n_{\uparrow}}{\omega_0 - U(n_{\uparrow} - n_{\downarrow})} \quad (441)$$

is solved by $\omega_0 = 0$. This is the beginning of a magnon branch. We can follow it by expanding Eq. (440) to quadratic order in \mathbf{q} , assuming that $\omega_{\mathbf{q}}$ is small compared to the gap Δ

$$\begin{aligned} 1 &= \frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q},\downarrow} - n_{\mathbf{k},\uparrow}}{\omega_{\mathbf{q}} - \epsilon_{\mathbf{k}+\mathbf{q},\downarrow} + \epsilon_{\mathbf{k},\uparrow}} \\ &\approx -\frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q},\downarrow} - n_{\mathbf{k},\uparrow}}{\epsilon_{\mathbf{k}+\mathbf{q},\downarrow} - \epsilon_{\mathbf{k},\uparrow}} - \omega_{\mathbf{q}} \frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q},\downarrow} - n_{\mathbf{k},\uparrow}}{(\epsilon_{\mathbf{k}+\mathbf{q},\downarrow} - \epsilon_{\mathbf{k},\uparrow})^2} \\ &\approx -\frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q},\downarrow} - n_{\mathbf{k},\uparrow}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + \Delta} - \omega_{\mathbf{q}} \left(-\frac{1}{\Delta} \right) \\ &\approx -\frac{U}{\Omega} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q},\downarrow} - n_{\mathbf{k},\uparrow}}{\Delta} \left[1 - \frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{\Delta} + \left(\frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{\Delta} \right)^2 \right] + \frac{\omega_{\mathbf{q}}}{\Delta} \\ &\approx 1 - \frac{U}{\Omega} \sum_{\mathbf{k}} \left[\frac{n_{\mathbf{k},\downarrow} + n_{\mathbf{k},\uparrow}}{\Delta^2} \frac{\mathbf{q}^2}{2m} - \frac{n_{\mathbf{k},\downarrow} - n_{\mathbf{k},\uparrow}}{\Delta^2} \frac{(2\mathbf{k} \cdot \mathbf{q})^2}{2m^2 \Delta} \right] + \frac{\omega_{\mathbf{q}}}{\Delta} \\ &\approx 1 + \frac{\mathbf{q}^2}{2m\Delta^2} \left(U n_0 - \frac{4\epsilon_F}{3} \right) + \frac{\omega_{\mathbf{q}}}{\Delta}. \end{aligned} \quad (442)$$

Solving for $\omega_{\mathbf{q}}$, this gives the dispersion

$$\omega_{\mathbf{q}} = \frac{\mathbf{q}^2}{2m\Delta} \frac{4\epsilon_F}{3} [UN(\epsilon_F) - 2] + \mathcal{O}(\mathbf{q}^4) \quad (443)$$

which we can rewrite as

$$\omega_{\mathbf{q}} \propto \mathbf{q}^2 \sqrt{\frac{U}{U_c} - 1}. \quad (444)$$

This form shows how the magnon dispersion is related to the Stoner instability and the dispersion becomes flat (the magnon heavy) near the transitions. That is, the magnons are very ‘soft’ or easy to excite near right after the symmetry-breaking transition. We recall that the magnon is the Goldstone mode of the continuously broken rotational symmetry.