Abstract

This is a LATEX template intended for academic theses, and was put together by Jabir Ali Ouassou while preparing his PhD dissertation. The template itself is released under a Creative Commons Attribution licence (CC BY 4.0). This basically means that you are free to use the template for any purpose as long as you give appropriate credit.

The template bundles the Libertinus fonts, which is used for all regular text and mathematics, and the URW classico fonts, which are used for chapter and section headings. The former is available under the Open Font Licence (SIL OFL 1.1), and is free for both private and commercial use. The latter is available under the Aladdin Free Public Licence (AFPL), and is only free for non-commercial use. If commercial use is of importance, a suitable replacement for URW classico would be the Libertinus Sans fonts, which are also bundled with the template.

Note that this template relies on LUALATEX for e.g. font customization, and on BIBTEX for reference handling. For command-line users, the easiest way to compile the document is to run `latexmk -lualatex thesis.tex`. If using an IDE, please check the program settings for how to enable compilation with LUALATEX and BIBTEX. The template is based on the KOMA-SCRIPT book class (`scrbook`), so for further customization of the template, please check out their documentation.

The template does not include a title page. This is because the style requirements typically varies between universities, and many institutions will anyway autogenerate a titlepage upon thesis submission.

Preface

This would be a natural place to specify what kind of thesis this is, acknowledge your supervisor and coworkers, and so on.

Contents

Introduction

In the world today we see an ever increasing need to not waste, but use energy in the form of electricity as efficiently as possible. There is also a continuous drive to create ever more advanced computers to process the ever increasing amounts of data that we produce and to help us calculate and come up with further innovation. At a fundamental level, the limit of how much advancement we can make in these areas is dependent on the materials available to build solutions out of and our understanding of how these materials behave. In the stone age, the material understanding allowed technology to be made out of wood, bone and stone. In the bronze age, technology superiour to this could be made because we had discovered how to extract a metal from its natural stony oxide. When it comes to solutions using electricity then the electrical properties of materials is naturally especially important. The current age has been called the information age, and most of the infrastructure upon which this information is stored and communicated through is possible because of our understanding of the behaviour of electricity, or more precicely electrons in materials. Electricity is understood as a stream of electrons and thus we often talk in this respect of materials electronic properties.

In 1911, the electronic property called superconductivity was discovered in Netherlands by Heike Onnes [1]. Mercury was cooled to $-268.99\,°\text{C}$ and then Dr. Onnes measured the resistivity, which is a measure of how much energy is used to push electrons through a ma-

terial. He found that the resistivity suddenly dissapeared at this temperature and lower. It was expected that the resistivity would become lower with temperature but the extreme suddenness of the dissapearance was surprising. Not only did resistivity dissapear so that electrons could flow completely freely through the material as if there was no material there at all, but in 1933 it was discovered that at this low temperature, its inside was devoid of any magnetic field, even if a magnetic field had previously penetrated the material at the higher temperatures. When a material changes its properties in such a sudden manner with respect to a controlling variable, in this case temperature, we call it a phase transition. Just as when the mechanical properties of water changes from making it easily fill the shape of a cup in its liquid form, to making it being stuck on top and impossible to drink after it has frozen into ice, so the electronic properties of mercury changes in a fundamental way as well during a phase transition. The phase transition that happens to water when it freezes into ice can be described by classical mechanics which is built on Newtons theories, however because of the Meissner effect, classical mechanics is not sufficient to describe the phase-transition that happens to mercury at $-268.99\,°C$. For that we need quantum mechanics. Thus the new low-temperature phase of mercury is not called a perfectly conducting phase, but a superconducting phase.

1.1 Climate Change and its solutions

Arguably one of modern industrialized civilization's largest future challenges is finding a way to reduce the amount of climate gases like carbon dioxide in the atmosphere.

Write an INTRODUCTION to the field field here.

Statistical Mechanics

In statistical mechanics we attempt to describe an ensemble of particles that may be interacting to extract not precise information about what each and every particle is doing, but statistical information about what most of the particles are doing. We zoom out and look upon the bunch of particles and try to answer the question of what is this bunch doing. What is the most significant behavior of this bunch as a whole.

2.1 Canonical ensamble and the partition function

Most of the business of statistical mechanics is about calculating what is known as the partition- function. Once this function is known, all the heavy lifting is done since most important statistical quantities can be extracted from it following already established systematic steps. To calculate the partition function is theoretically very simple: we sum the quantity $e^{-\beta E_i}$ over all the possible states of the system. Every state is a particular configuration of things in the system and since all things in the system has a certain energy, if we sum the energy of all the things in the system for each state, we can say that each state has a certain energy. If we label each state of the system with the index i, then we can denote the energy of each state E_i. The definition of the partition function Z in the canonical ensamble can then be written

$$Z = \sum_i e^{-\beta E_i},$$

(2.1)

where $\beta = 1/(k_{\mathrm{B}}T)$ and k_{B} is the Boltzmann constant given by $k_{\mathrm{B}} \approx 1.380\,649 \times 10^{-23}\,\mathrm{JK}^{-1}$.

As we can see, the essential ingredients needed to calculate the partition function is to be able to enumerate all possible states i of the system and also calculate their corresponding energy E_i. Since we have used the summation sign $\sum_i$ in Eq. (2.1), we have implicitly assumed that there exists a finite number of different states. However if there is one thing in the system that can change in a continuous fashion, which we would measure using the set of real numbers $\mathbb{R}$ and some unit, then the number of states is infinite. In this case we sum over the different numbers of states by simply integrating over the things that are continuous and the unit of the partition function becomes the product of the units of the continuous variables (things). In most cases, it is the position and momentum of particles in the system that are continuous, hence the definition of the partition function becomes[1]

$$Z \sim \int \mathrm{d}^3 r \int \mathrm{d}^3 p \, e^{-\beta E(\boldsymbol{r}, \boldsymbol{p})}. \tag{2.2}$$

2.2 Calculating observables

An observable in statistical mechanics is anything that we want to measure. In quantum mechanics observables are restricted to operators that have real eigenvalues which makes sense considering that we don't really have an intuition for complex numbers, which is the alternative, and thus we want to restrict things we can observe to things we can understand in terms of a point on a single line (the real axis).

Since we are interested again in ensembles of many particles we are restricting our attention to statistical information about this ensamble. To get this information we need some kind of probability distribution of the particular states of the system. We are imagining that we for each such state (indexed by j) can calulate a real number for the thing (observable) we are interested in measuring. Let's call this observable O. Then O is a statistical variable but takes a particular value o_j in the state j of the system. If we now let P_j be the probability distribution,

---

1. The reason why there is a $\sim$ sign in Eq. (2.2) is that specifically there is a factor of Planck's constant h in the denominator for each $\mathrm{d}r\,\mathrm{d}p$ in the integral measure since this makes the partition function dimensionless and thus consistent with the definition in terms of finite number of states.

i.e. the probability that the system exists in state j, then we know from probability theory that the mean of the observaible is

$$\langle O \rangle = \sum_j o_j P_j. \tag{2.3}$$

The probability distribution P_j is given by

$$P_j = e^{-\beta E_j}/Z, \tag{2.4}$$

in terms of the partition function Z. Inserting this we get

$$\langle O \rangle = \sum_j \frac{o_j e^{-\beta E_j}}{Z}. \tag{2.5}$$

2.3 Ginzburg-Landau model

The experimental discovery of superconductivity was a surprise to the scientists at the time. No theoretical model had so far predicted the properties that the experimentalists were measuring. On the contrary, they predicted very different results no matter how they were twisted and turned, and thus superconductivity seemed to demand a radically different understanding of how electrons moved in a material.

2.3.1 Landau Model

Before such an understanding had been developed, Landau took a shortcut and came up with a theory that could describe the phenomenon of superconductivity without knowing its microscopic origin. In other words he treated superconductivity as a black box and instead of asking what was inside to give the boxes output, he used the output to determine a small set of *material parameters* which could then be used to predict how the box would react to a large range of stimuli or conditions. The merit of the theory was that he used symmetry arguments to reduce this set as much as possible.

The Ginzburg-Landu theory of superconductivity is based on Landau's previous work on a theory for general second order phase-transitions[2]

---

2. 2nd order phase-transitions are phase transitions of systems whose free energy has a discontinuous second order derivative at the transition point, but is continuous for lower orders. Since the specific heat is given by the second order derivative, then the specific heat is discontinuous in this case.

The approach is given by two ideas. The first is simply that the phase transition should be able to be characterized by the appearence of some kind of measurable order that can be described by a function ψ which we call the *order parameter*. In the liquid water to ice transition, it is the position of the molecules that become ordered in a lattice,[3] in the magnetization of a metal it is the individual spins that become ordered along a particular direction.

The second idea is that at the phase transition, it is the appearance of this order that should dominate the behaviour of the system, to the exclusion of all other effects. Thus the system should be described in terms of the order-parameter and since this is infinitesimally small close to the transition, the free energy[4] can be expanded in a Maclaurin-series with respect to this parameter as

$$F = F_0 + c_1\psi + c_2\psi^2 + c_3\psi^3 + c_4\psi^4 + c_5\psi^5 + \ldots \qquad (2.6)$$

The real constants F_0 and c_i constitute the set of material parameters of the theory and this set can then be reduced by any symmetries that we suspect should be inherent in the underlying theory. For example, if ψ should represent the order parameter of magnetization of a system of ising spins, which can point either up or down, then the free energy should be invariant of this global choice, i.e. we need to enforce that the free energy be invariant with respect to the transformation $\psi \mapsto -\psi$. Then all the constants c_j for odd j vanish.

In the case of superconductivity the order parameter Ψ represents the probability amplitude of the collective state of the superfluid of Cooper paired electrons such that $|\Psi|$ can be interpreted as the density of such electron pairs. Since Ψ is complex it has to be combined with its complex conjugate Ψ^* in ways that yield real numbers to produce terms that are valid in the free energy since F itself should be a real number. Furthermore, the phenomenon of superconductivity is produced as a result of the breaking of $U(1)$ symmetry, so F needs

---

3. The astute reader might have noticed that this example is a first order phase transition because of the existance of latent heat. Actually first order phase transitions is also able to be described by a modified Landau theory, however we will here focus on the second order kind.

4. In this case we are talking about the Helmholtz free energy which is related to the partition function through a logarithm while at the same time the Legendre transformation of the internal energy of the thermodynamic system.

also to be $U(1)$ symmetric, i.e. it has to be invariant under the transformation $\Psi \mapsto e^{i\phi}\Psi$ for $\phi \in \mathbb{R}$. These restrictions result in the free energy

$$F = F_0 - a|\Psi|^2 + b|\Psi|^4, \qquad (2.7)$$

when keeping the lowest order terms that produce a phase transition.

Thermodynamic equilibrium is reached at the minimum of free energy. This restricts $b \geq 0$ since negative b yields a free energy with no definite minimum. The minimum is then found by the condition

$$\frac{\partial F}{\partial \Psi^*} = (-a + 2b|\Psi|^2)\Psi = 0, \qquad (2.8)$$

which yields the possibilities $|\Psi| = 0$ or $|\Psi| = \sqrt{a/2b}$. The first case gives the energy $F = F_0$, while the second gives $F = F_0 - a^2/(4b)$. We see that the second case is energetically favorable, but only exists and is different from the first case when $a > 0$. Furthermore, the second case represents the ordered state since in this case the order-parameter $|\Psi| \neq 0$, in the conventional Landau theory.[5]

In superconductivity it is the parameter of temperature which conventionally determines when the system enters the superconducting regime. Looking at the free energy in Eq. (2.7), the order parameter Ψ is the dynamical variable of the theory while the explicit temperature dependence lies in the material parameters a and b. Denoting the temperature at which the phase transition happens — the critical temperature: T_c, the dimensionless parameter $t = (T - T_c)/T_c$ is small close to the critical point which means it can be used to expand the temperature dependence of the material parameters such that

$$\begin{aligned} a(T) &= a_0 + a_1 t + ... \\ b(T) &= b_0 + b_1 t + ... \end{aligned} \qquad (2.9)$$

Now we argue for what terms to keep in these expansions. Since $a(T)$ should change sign at $t = 0$ then we only keep odd terms. Since

---

5. Actually this only represents when Cooper-pairs are forming and the real onset of superconductivity is determined by the point in parameter-space where the gauge-mass becomes non-zero, which is closely related but not exactly the same as where the density of Cooper-pairs becomes non-zero. The real onset of superconductivity is thus more related to when the phase of the wave-function settles on a value.

we need $b(T) > 0$ for the theory to be thermodynamically stable it seems that b_0 is the important term which need to be larger than any negative contributions from the other terms. Keeping only lowest order terms then the expansions reduce to $a(T) = a_1(T - T_c)/T_c$ and $b(T) = b_0$. Since the ordered state is the solution of the theory when $a > 0$ and this ordered state exists at temperatures $T < T_c$ then $a_1 < 0$ and the final temperature dependence of a becomes $a(T) = -|a_1|(T - T_c)/T_c$. From this temperature dependence, it is straight forward to derive critical exponents, the specific heat etc.

2.3.2 Gradient Terms

The simple Landau theory described above is a type of mean field theory in that there is no spatial dependence in the solution, and thus gives a simplified picture that can only be valid far away from any defects or boundaries. This simple approach can be extended to include spatial variation by allowing terms with gradients of the order parameter in the free energy through a gradient expansion

$$F = \int \mathrm{d}^3 r \; f(\Psi, \nabla\Psi, \nabla^2\Psi, \nabla^3\Psi, ...). \qquad (2.10)$$

Keeping only the lowest order in this expansion that is invariant under $U(1)$ symmetry we get the term $|\nabla\Psi|^2$.

Perhaps the single most important phenomenon of superconductivity from a theoretical stand-point is the fact that it expells magnetic fields, hence it is clear that any theory that attempts to explain superconductivity needs to have some way the superconducting order interacts with magnetic fields. The standard way to acheive this is through the recipe of *minimal coupling*, where the vector potential $\boldsymbol{A}$ times a constant is subtracted with from any momentum in the previously neutral theory. Specifically $\boldsymbol{p} \mapsto \boldsymbol{p} - q/c\boldsymbol{A}$ where q is the charge of the particle and c is the speed of light.

$$f = f_0 - a|\Psi|^2 + b|\Psi|^4 + K|(\nabla + ig\boldsymbol{A})\Psi|^2 - \int_0^{B_a} \boldsymbol{M} \cdot \mathrm{d}\boldsymbol{B}_a \quad (2.11)$$

<++>

CHAPTER 3

Field Theory Methods

In this chapter we will give a short introduction to the use of grassmann variables and complex numbers in the calculation of the field-integrals on the statistical-mechanical partition function and how they can be used to transform the expression for the action through the Hubbard-Stratonovich transformation.

3.1 Pfaffian

3.2 Hubbard-Stratonovich transformation

3.3 Extended Nambu notation

3.4 Log-expansion

Group Theory

In this chapter we will introduce the minimum mathematical framework needed to understand the phrase "This free energy is the Γ_{5u}^{-} irreducible representation of the D_{4h} symmetry group".

A few words about notation. We will use the semicolon ';' in equations as notation for the words 'such that', e.g. when defining sets. A colon ': ' is used when defining maps where the symbol representing the mapping itself should be on the left while the the sets being related or how the elements of the sets are related is on the right of the colon. The colon ':' is also used as a shortcut for the words 'applied through its representation to' for when group elements are applied to vectors, where the correct representation to use for this application should be implicitly understood.

4.1 Discrete groups

4.2 Irreducible representations

To know what an irreducible representation is, let's start with what we mean by a reducible representation.

Def. 4.1. *A matrix representation is **reducible** if there exists a non-trivial invariant subspace of the vector space of the representation.*

The intuition is then that the vector space of the representation is reducible if a "smaller" representation is contained within it. Since

there is a smaller vector space within the vector space of the original representation and this vector space is invariant, it is possible to define another representation on this smaller vector space, i.e. *reduce* the original representation. We have now used the word "invariant" a couple of times, so let's define what it means more precisely.

Def. 4.2. *Let $D(g)$ a representation of the group G on the vector space V such that $D(g)\colon V \to V$. Then a subspace $U \subseteq V$ is **invariant** if*

$$\forall g \in G \quad u \in U \implies D(g)u \in U. \tag{4.1}$$

In other words: a vector space is invariant if it is not possible for any vector in it to escape using a representation of any group element. All representations applied to any vector in the invariant subspace must necessarily land in that same subspace from which it started.

Thm. 4.1 (Shur's Lemma). *If $D(g)$ is an irreducible complex representation with vector space V and $L(V)$ is the set of all linear maps, then*

$$\{A \in L(V);\ AD(g) = D(g)A\ \forall g \in G\} = \{c\mathbb{1};\ c \in \mathbb{C}\}. \tag{4.2}$$

4.3 BCS Hilbert Space

We define the BCS Hilbert space as the Hilbert space upon which BCS-type potentials operate. Specifically this is a reduced form of the two-state fermionic product Hilbert space $\mathcal{H}_2 = \mathcal{H} \otimes \mathcal{H}$ where $\mathcal{H} = \mathrm{span}\{|\boldsymbol{k}, s\rangle\}$ and we only consider states that have opposite momentum. Thus this Hilbert space is given by

$$\mathcal{B} = \mathrm{span}\{|\boldsymbol{k}, s_1\rangle|-\boldsymbol{k}, s_2\rangle\}, \tag{4.3}$$

and the identity operator in this space can be written

$$\hat{\mathbb{1}} = \sum_{\boldsymbol{k}\, s_1 s_2} |\boldsymbol{k}, s_1\rangle|-\boldsymbol{k}, s_2\rangle\langle-\boldsymbol{k}, s_2|\langle\boldsymbol{k}, s_1|. \tag{4.4}$$

Acting on the arbitrary vector $|v\rangle \in \mathcal{B}$ with this identity operator, we find that in terms of this basis it can be written

$$|v\rangle = \sum_{\boldsymbol{k}\, s_1 s_2} v_{s_1 s_2}(\boldsymbol{k})|\boldsymbol{k}, s_1\rangle|-\boldsymbol{k}, s_2\rangle, \tag{4.5}$$

where

$$v_{s_1 s_2}(\boldsymbol{k}) = \langle -\boldsymbol{k}, s_2 | \langle \boldsymbol{k}, s_1 \mid v \rangle. \tag{4.6}$$

The indices s_1 and s_2 can take on only two values each, namely $s_1, s_2 \in \{\uparrow, \downarrow\}$. In total there are thus 4 different realizations of pairs, $s_1 s_2$ e.g. $\uparrow\uparrow$ for $v_{s_1 s_2}(\boldsymbol{k})$. Putting these different realizations of $v_{s_1 s_2}(\boldsymbol{k})$ as elements in a 2×2 matrix we get

$$v_{s_1 s_2}(\boldsymbol{k}) = \begin{pmatrix} v_{\uparrow\uparrow}(\boldsymbol{k}) & v_{\uparrow\downarrow}(\boldsymbol{k}) \\ v_{\downarrow\uparrow}(\boldsymbol{k}) & v_{\downarrow\downarrow}(\boldsymbol{k}) \end{pmatrix}. \tag{4.7}$$

Any 2×2 matrix can be written in the conventional basis of the 4 Pauli matrices $\sigma^0 = \mathbb{1}_{2\times 2}$, σ^x, σ^y, and σ^z. This means that we could write the matrix in Eq. (4.7)

$$v_{s_1 s_2}(\boldsymbol{k}) = v_{\boldsymbol{k}}^0 \sigma_{s_1 s_2}^0 + v_{\boldsymbol{k}}^i \sigma_{s_1 s_2}^i. \tag{4.8}$$

It is however conventional to factor out a Pauli matrix $i\sigma^y$ to the right in the expansion since this results in nice transformation properties of the coefficients as we shall see. With the spin-indices expanded in this basis it is conventional to let the function of $\boldsymbol{k}$ that is in front of σ^0 be called $\psi_{\boldsymbol{k}}$. The three others are conventionally denoted $d_{\boldsymbol{k},i}$. Expanded in this conventional basis then $v_{s_1 s_2}(\boldsymbol{k})$ takes the form

$$v_{s_1 s_2}(\boldsymbol{k}) = (\psi_{\boldsymbol{k}} \sigma_{s_1 s'}^0 + d_{\boldsymbol{k},i} \sigma_{s_1 s'}^i) i\sigma_{s' s_2}^y, \tag{4.9}$$

and finally the state $|v\rangle$ can be written

$$|v\rangle = \sum_{\boldsymbol{k} s_1 s_2} [(\psi_{\boldsymbol{k}} \sigma^0 + \boldsymbol{d}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}) i\sigma^y]_{s_1 s_2} |\boldsymbol{k}, s_1\rangle |-\boldsymbol{k}, s_2\rangle. \tag{4.10}$$

Going one step back and writing out the different combinations of $s_1 s_2$ in $v_{s_1 s_2}(\boldsymbol{k})$ as a matrix like we did in Eq. (4.7), but now multiplying out the Pauli matrices in Eq. (4.9) we get

$$\begin{pmatrix} v_{\uparrow\uparrow}(\boldsymbol{k}) & v_{\uparrow\downarrow}(\boldsymbol{k}) \\ v_{\downarrow\uparrow}(\boldsymbol{k}) & v_{\downarrow\downarrow}(\boldsymbol{k}) \end{pmatrix} = \begin{pmatrix} -d_{\boldsymbol{k},x} + id_{\boldsymbol{k},y} & \psi_{\boldsymbol{k}} + d_{\boldsymbol{k},z} \\ -\psi_{\boldsymbol{k}} + d_{\boldsymbol{k},z} & d_{\boldsymbol{k},x} + id_{\boldsymbol{k},y} \end{pmatrix}. \tag{4.11}$$

This set of linear relations is easily inverted to yield

$$\psi_{\boldsymbol{k}} = \frac{1}{2}(v_{\uparrow\downarrow}(\boldsymbol{k}) - v_{\downarrow\uparrow}(\boldsymbol{k})) \tag{4.12}$$

$$d_{\boldsymbol{k},x} = \frac{1}{2}(v_{\downarrow\downarrow}(\boldsymbol{k}) - v_{\uparrow\uparrow}(\boldsymbol{k})) \tag{4.13}$$

$$d_{\boldsymbol{k},y} = -\frac{i}{2}(v_{\uparrow\uparrow}(\boldsymbol{k}) + v_{\downarrow\downarrow}(\boldsymbol{k})) \tag{4.14}$$

$$d_{\boldsymbol{k},z} = \frac{1}{2}(v_{\uparrow\downarrow}(\boldsymbol{k}) + v_{\downarrow\uparrow}(\boldsymbol{k})). \tag{4.15}$$

Since the space $\mathcal{B}$ is fermionic we have the symmetry

$$|\boldsymbol{k}, s_1\rangle|-\boldsymbol{k}, s_2\rangle = -|-\boldsymbol{k}, s_2\rangle|\boldsymbol{k}, s_1\rangle. \tag{4.16}$$

Using this symmetry transformation on the basis vectors in the expansion of $|v\rangle$ in Eq. (4.6), then renaming indices and finally equating coefficients term by term, we see that for the coefficients of $|v\rangle$, this symmetry takes the form

$$v_{s_1 s_2}(\boldsymbol{k}) = -v_{s_2 s_1}(-\boldsymbol{k}). \tag{4.17}$$

4.4 Application of group elements

When we are talking about applying some symmetry transformation to a state, this is synonymous with applying a group element to a vector. Even more specifically, the 'applying' part means that we have some natural representation of the group on the vector space we have defined states on, and we are using the linear transformation of the representation of the group element to act on the state vector. In this thesis we will use the notation $g : |\psi\rangle$ to refer to this procedure.

Let g be an arbitrary group element in the symmetry group G and D be a representation of G on the d-dimensional vector space V. Let V have a basis $\{\boldsymbol{b}_i\}_{i=1}^d$. The application of a group element to a basis vector is then defined as

$$g : \boldsymbol{b}_i = \sum_j \boldsymbol{b}_j D_{ji}(g). \tag{4.18}$$

The application of a group element to any vector in V then is calculated by expanding the vector in the basis and applying the representation D to each basis vector separately as a linear transformation:

$$g : \boldsymbol{v} = \sum_i v_i g : \boldsymbol{b}_i. \tag{4.19}$$

4.4.1 Active vector transformation

As g : has been defined in Eq. (4.18) it is defined in a passive perspective where the transformation is happening to the basis vectors. Applying g to a vector $\boldsymbol{v}$ in the basis $\{\boldsymbol{b}_i\}$ it is sometimes useful to consider this as an application not on the vectors themselves but on the expansion coefficients v_i of $\boldsymbol{v}$ in the basis. This is the active view of the transformation. Inserting Eq. (4.18) into Eq. (4.19) we get

$$
\begin{aligned}
g : \boldsymbol{v} &= \sum_i v_i \sum_j \boldsymbol{b}_j D_{ji}(g) = \sum_j \left(\sum_i D_{ji}(g) v_i \right) \boldsymbol{b}_j \\
&= \sum_i v_i' \boldsymbol{b}_i,
\end{aligned}
\tag{4.20}
$$

where we have defined the transformed coefficients

$$
v_i' = \sum_j D_{ij}(g) v_j.
\tag{4.21}
$$

From this calculation we see that we can consider the application of g as a transformation of the coefficients of the vector as

$$
g : v_i = \sum_j D_{ij}(g) v_j.
\tag{4.22}
$$

This defines the active transformation of a vector v by a group element g.

4.4.2 Representation on product spaces

The product space $V \otimes V$ then has a basis $\{\boldsymbol{b}_i \boldsymbol{b}_j\}_{i,j=1}^d$. A derived representation can be constructed from D on this product space called the product representation $D^{(D \times D)}(g)$. This is defined through its application on the basis by

$$
g : \boldsymbol{b}_i \boldsymbol{b}_j = \sum_{kl} \boldsymbol{b}_k \boldsymbol{b}_l \left[D^{(D \times D)}(g) \right]_{kl,ij} = \sum_{kl} \boldsymbol{b}_k \boldsymbol{b}_l D_{ki}(g) D_{lj}(g).
\tag{4.23}
$$

To apply group theory to physical problems, we need to know how the objects we are working with in the physical theory transform under group elements. The most important vector space in quantum mechanics is arguably the Hilbert space where particle states are determined by a momentum and spin quantum number. Each quantum

number has its own vector space defined by the basis vectors $|\mathbf{k}\rangle$ and $|s\rangle$ in the Dirac notation. The combination of both quantum numbers in the description of a particle state then gives a state in the product space of these vector spaces. A basis for this space is given by the vectors $|\mathbf{k}, s\rangle = |\mathbf{k}\rangle|s\rangle$. Given $\mathbf{k} \in \mathbb{R}^d$ and $s \in \{\uparrow, \downarrow\}$, these basis vectors transform according to the product representation of the representations on each vector space, given by

$$g : |\mathbf{k}', s'\rangle = \sum_{\mathbf{k}s} |\mathbf{k}, s\rangle D^{(\mathbf{k}\times s)}_{\mathbf{k}s;\, \mathbf{k}'s'} = \sum_{\mathbf{k}s} |\mathbf{k}, s\rangle D_{g\, ss'} \delta_{\mathbf{k}, g:\mathbf{k}'}, \quad (4.24)$$

under a group element g. Here $g\mathbf{k}'$ means application of g to the vector $\mathbf{k}'$ through the standard representation of g in $\mathbb{R}^d$. $D_{g\, ss'}$ is a representation on the spin-up spin-down vector space given by the matrix

$$D_{g\, ss'} = \sigma^0_{ss'} \cos(\phi/2) - i\hat{\mathbf{u}} \cdot \boldsymbol{\sigma}_{ss'} \sin(\phi/2), \quad (4.25)$$

where $\hat{\mathbf{u}}$ is the rotation axis unity vector, while ϕ is the angle that defines the proper rotation associated with g. $\boldsymbol{\sigma}$ is the vector notation for the 3 Pauli matrices and $\sigma^0_{ss'} = \delta_{ss'}$.

In the BCS Hilbert space which we discussed in more detail in Section 4.3, the basis vectors are outer products of the momentum spin basis vectors with opposite momentum: $\{|\mathbf{k}, s_1\rangle|-\mathbf{k}, s_2\rangle\}$. The product representation on this vector space then transforms the basis vectors according to

$$g : |\mathbf{k}', s'_1\rangle|-\mathbf{k}', s'_2\rangle = \sum_{\mathbf{k}\, s_1 s_2} |\mathbf{k}, s_1\rangle|-\mathbf{k}, s_2\rangle D^{(D\times D)}_{\mathbf{k}\, s_1 s_2;\, \mathbf{k}'\, s'_1 s'_2}(g),$$

$$(4.26)$$

where

$$D^{(D\times D)}_{\mathbf{k}\, s_1 s_2;\, \mathbf{k}'\, s'_1 s'_2}(g) = D_{g\, s_1 s'_1} \delta_{\mathbf{k}, g:\mathbf{k}'} D_{g\, s_2 s'_2} \delta_{-\mathbf{k}, g:-\mathbf{k}'}. \quad (4.27)$$

Since group representations on $\mathbf{k}$ is a linear transformation then $\delta_{-\mathbf{k}, g:-\mathbf{k}'} = \delta_{\mathbf{k}, g:\mathbf{k}'}$, such that the last Kronecker delta function becomes superfluous.

4.4.3 Representation on ψ-$\boldsymbol{d}$ functions

The coefficients of the basis expansion of a vector in the BCS Hilbert space were given in the conventional ψ-$\boldsymbol{d}$ notation in Eq. (4.10). Taking

the active view of group transformations we can say that the expansion coefficients of arbitrary states in the BCS Hilbert space $\mathcal{B}$ transforms like the v_i in Eq. (4.22) but where now the representation matrix D is given by the matrix $D^{(D\times D)}_{\boldsymbol{k}\,s_1 s_2;\,\boldsymbol{k}'\,s_1' s_2'}$ above in Eq. (4.27). Written out then, the coefficients transform according to

$$g : v_{s_1 s_2}(\boldsymbol{k}) = \sum_{\boldsymbol{k}'\,s_1' s_2'} D^{(D\times D)}_{\boldsymbol{k}\,s_1 s_2;\,\boldsymbol{k}'\,s_1' s_2'} v_{s_1' s_2'}(\boldsymbol{k}'). \tag{4.28}$$

Let now $|v\rangle$ be a state that is even in space, meaning that its expansion only consists of coefficients $\psi(\boldsymbol{k})$ in the ψ-$\boldsymbol{d}$ notation. Then we see from Eq. (4.11) that $\psi(\boldsymbol{k})$ can be written $\psi(\boldsymbol{k}) = v_{\uparrow\downarrow}(\boldsymbol{k})$. The transformation properties of $\psi(\boldsymbol{k})$ are thus given by

$$g : \psi(\boldsymbol{k}) = g : v_{\uparrow\downarrow}(\boldsymbol{k}) = \sum_{\boldsymbol{k}'\,s_1' s_2'} D^{(D\times D)}_{\boldsymbol{k}\uparrow\downarrow;\,\boldsymbol{k}'\,s_1' s_2'} \psi(\boldsymbol{k}')(i\sigma^y)_{s_1' s_2'}$$
$$= \psi(g^{-1} : \boldsymbol{k})(i\sigma^y)_{\uparrow\downarrow} = \psi(g^{-1} : \boldsymbol{k}). \tag{4.29}$$

In this calculation we inserted the expression of $D^{(D\times D)}_{\boldsymbol{k}\,s_1 s_2;\,\boldsymbol{k}'\,s_1' s_2'}$ in Eq. (4.27) and used the equation $D_g i\sigma^y D_g^\mathsf{T} = i\sigma^y$, where D_g are the spin representation matrices given in Eq. (4.25).

To find the transformation properties of $\boldsymbol{d_k}$ the principle is the same as above for $\psi(\boldsymbol{k})$ but the calculations become more involved. We assume that the spin-momentum basis expansion of state $|v\rangle$ consists of only odd coefficients so that $v_{s_1 s_2}(\boldsymbol{k}) = \boldsymbol{d_k} \cdot (\boldsymbol{\sigma} i\sigma^y)_{s_1 s_2}$. Inserting this into the active transformation of the coefficients of $|V\rangle$ in Eq. (4.28) and also inserting the expression for $D^{(D\times D)}_{\boldsymbol{k}\,s_1 s_2;\,\boldsymbol{k}'\,s_1' s_2'}$ as we did before yields

$$g : v_{s_1 s_2}(\boldsymbol{k}) = \sum_{\boldsymbol{k}'\,s_1' s_2'} \delta_{\boldsymbol{k},g:\boldsymbol{k}'} D_{g\,s_1 s_1'} D_{g\,s_2 s_2'} \boldsymbol{d_{k'}} \cdot (\boldsymbol{\sigma} i\sigma^y)_{s_1' s_2'}$$
$$= \sum_s \left(D_g \boldsymbol{\sigma} \sigma^y D_g^\mathsf{T} \sigma^y \right)_{s_1 s} \cdot \boldsymbol{d}_{g^{-1}:\boldsymbol{k}}\, i\sigma^y_{s s_2}. \tag{4.30}$$

Since a group transformation (aka. the linear transformation given by a group representation) can not bring a state that was even to be odd or vice versa, then the resulting state given by the transformed coefficients $g : v_{s_1 s_2}(\boldsymbol{k})$ has to remain odd, and thus they can be expanded in terms of a new $\boldsymbol{d}'$ such that

$$g : v_{s_1 s_2}(\boldsymbol{k}) = \sum_s \boldsymbol{d}'_{g^{-1}:\boldsymbol{k}} \cdot \boldsymbol{\sigma}_{s_1 s} i\sigma^y_{s s_2}. \tag{4.31}$$

Having expanded both sides of the transformed coefficients with a common factor $i\sigma^y$ to the right we can equate the remaining 2×2 spin matrices which gives an expression for $\boldsymbol{d}'_{g^{-1}:\boldsymbol{k}} \cdot \boldsymbol{\sigma}$ by comparing Eq. (4.30) and Eq. (4.31). Furthermore, using the anti-commutation property $\{\sigma^i, \sigma^j\} = 2\delta_{ij}\sigma^0$ of Pauli matrices we find that

$$d'_{\boldsymbol{k},i} = \frac{1}{4} \operatorname{Tr}\left(\{\sigma^i, \boldsymbol{d}'_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}\}\right). \tag{4.32}$$

Inserting the expression for $\boldsymbol{d}'_{g^{-1}:\boldsymbol{k}} \cdot \boldsymbol{\sigma}$ and the full expression of the $SU(2)$ spin-representation matrices D_g, which is found in Eq. (4.25), yields after some algebra

$$
\begin{aligned}
d'_{g^{-1}:\boldsymbol{k},i} &= \frac{1}{4} \operatorname{Tr}\left(\{\sigma^i, \boldsymbol{d}_{g^{-1}:\boldsymbol{k}} \cdot D_g \boldsymbol{\sigma} \sigma^y D_v^\mathsf{T} \sigma^y\}\right) \\
&= R_{ij}(\hat{\boldsymbol{u}}, \phi) d_{g^{-1}:\boldsymbol{k},j},
\end{aligned}
\tag{4.33}
$$

where we have defined the matrix

$$R_{ij}(\hat{\boldsymbol{u}}, \phi) = \delta_{ij} \cos\phi + \hat{u}_i \hat{u}_j (1 - \cos\phi) - \epsilon_{ijk} \hat{u}_k \sin\phi$$

$$= \begin{pmatrix} \cos\phi + \hat{u}_x^2(1-\cos\phi) & \hat{u}_x\hat{u}_y(1-\cos\phi) - \hat{u}_z\sin\phi & \hat{u}_x\hat{u}_z(1-\cos\phi) + \hat{u}_y\sin\phi \\ \hat{u}_y\hat{u}_x(1-\cos\phi) + \hat{u}_z\sin\phi & \cos\phi + \hat{u}_y^2(1-\cos\phi) & \hat{u}_y\hat{u}_z(1-\cos\phi) - \hat{u}_x\sin\phi \\ \hat{u}_z\hat{u}_x(1-\cos\phi) - \hat{u}_y\sin\phi & \hat{u}_z\hat{u}_y(1-\cos\phi) + \hat{u}_x\sin\phi & \cos\phi + \hat{u}_z^2(1-\cos\phi) \end{pmatrix}.$$

$$\tag{4.34}$$

This matrix is in fact the rotation matrix of a vector in $\mathbb{R}^3$ by an angle ϕ about a unit vector $\hat{\boldsymbol{u}}$. Since the coefficients of an odd state $|v\rangle$ are fully determined by the vector $\boldsymbol{d}$, their transformation can be regarded just as a tranformation of $\boldsymbol{d}$ itself which thus takes the form

$$g : d_{\boldsymbol{k},i} = R_{ij}(\hat{\boldsymbol{u}}, \phi) d_{g^{-1}:\boldsymbol{k},j}, \tag{4.35}$$

where $\hat{\boldsymbol{u}}$ and ϕ gives the unit vector and angle respectively, of the proper rotation associated with g. The conclusion is thus that $\boldsymbol{d}$ transforms as a vector by the proper rotation associated with g.

4.4.4 Projection Operators

Let us assume that we are in a vector space V that can be divided into possibly several different irreducible representations $D^{(\alpha)}$ of some symmetry group G. Further, let the basis vectors of these irreducible

representations be denoted by $\boldsymbol{b}_m^{(\alpha)}$ where m thus counts the number of basis vectors in each irrep. Then an arbitrary vector $\boldsymbol{f} \in V$ can be written in terms of these basis vectors as

$$\boldsymbol{f} = \sum_\alpha \sum_m c_m^{(\alpha)} \boldsymbol{b}_m^{(\alpha)}. \tag{4.36}$$

A projection operator can be used to extract any combination of constant $c_m^{(\alpha)}$ multiplied by a basis vector $\boldsymbol{b}_n^{(\alpha)}$, where m and n can in general be different. Denoting the projection operator that picks out the mth constant multiplied by the lth basis vector in the irrep. β of the expansion of $\boldsymbol{f}$: $P_{lm}^{(\beta)}$, then

$$P_{lm}^{(\beta)} \boldsymbol{f} = c_m^{(\beta)} \boldsymbol{b}_l^{(\beta)}. \tag{4.37}$$

This is extremely useful in finding a bases for the irreducible representations. To acheive this, the projection operator is defined as

$$P_{l,m}^{(\beta)} = \frac{d_\beta}{|G|} \sum_{g \in G} D_{lm}^{(\beta)}(g)^* g :, \tag{4.38}$$

where d_β is the dimension of irrep. β, $D_{lm}^{(\beta)}(g)$ is the lm element of the matrix representation of the group element g and finally we have used the notation $g :$ to denote application on vectors by the relevant representation. An example is the application of g to the basis vectors $\boldsymbol{b}_m^{(\alpha)}$. Since the relevant representation of g in this case is the irreducible representation for which $\boldsymbol{b}_m^{(\alpha)}$ is a basis vector, the application becomes

$$g : b_m^{(\alpha)} = \sum_n b_n^{(\alpha)} D_{nm}^{(\alpha)}(g). \tag{4.39}$$

Usually, the full generality of the projection operators $P_{l,m}^{(\beta)}$ isn't needed and it suffices to consider the diagonal projection operators $P_{l,l}^{(\beta)} \equiv P_l^{(\beta)}$ or indeed their sum, in which case the resulting operator can be written only in terms of the irrep. characters $\chi^{(\alpha)}(g)$ since

$$P^{(\beta)} \equiv \sum_l P_l^{(\beta)} = \frac{d_\beta}{|G|} \sum_{g \in G} \sum_l D_{ll}^{(\beta)}(g)^* g := \frac{d_\beta}{|G|} \sum_{g \in G} \chi^{(\beta)}(g)^* g : . \tag{4.40}$$

4.5 Fermionic symmetry transformations

4.6 Time-reversal symmetry

4.7 Symmetries of the Square Lattice

The symmetry group of the square lattice is denoted C_{4v} in the Schön-flies notation. It contains 8 elements in total:

e: The identity element (do nothing),

C_4: Rotation by $90°$ in the positive direction (ccw),

C_4^{-1}: Rotation by $90°$ in the negative direction (cw),

C_4^2: Rotation by $180°$,

σ_x: Mirror about the zy-plane,

σ_y: Mirror about the zx-plane,

σ_{d_1}: Mirror about the downwards diagonal plane,[1]

σ_{d_2}: Mirror about the upwards diagonal plane.

This results in the group multiplication table in Table 4.1. We can check that this is correct by performing the group transformations in the top row followed by the one in the left column and seeing that this results in the group transformations where these two intersect. As an example consider the vector $(x, y)^\mathsf{T}$. Transforming this by the $90°$ counter clockwise rotation C_4 we get $(-y, x)^\mathsf{T}$. Then mirroring this result about the yz-plane yields $(y, x)^\mathsf{T}$. We now realize that this is the same as mirroring the original vector about the axis $y = x$, hence $\sigma_x C_4 = \sigma_{d_2}$ as the multiplication table says.

The conjugation classes of a group is the sets of group elements that is conjugate to each other, meaning that there exists a group element g such that $gAg^{-1} = B$ between conjugate elements A and B. Since conjugation is an equivalence relation it subdivides the group elements exactly into conjugation classes. The conjugation classes of the group C_{4v} are $e = \{e\}$, $2C_4 = \{C_4, C_4^{-1}\}$, $C_4^2 = \{C_4^2\}$, $2\sigma_d = \{\sigma_{d_1}, \sigma_{d_2}\}$

---

1. We are assuming the western bias of left-to-right movement here. More precisely it is the plane containing the z axis and the axis $y = -x$

	e	C_4	C_4^2	C_4^{-1}	σ_x	σ_y	σ_{d_1}	σ_{d_2}
e	e	C_4	C_4^2	C_4^{-1}	σ_x	σ_y	σ_{d_1}	σ_{d_2}
C_4	C_4	C_4^2	C_4^{-1}	e	σ_{d_1}	σ_{d_2}	σ_y	σ_x
C_4^2	C_4^2	C_4^{-1}	e	C_4	σ_y	σ_x	σ_{d_2}	σ_{d_1}
C_4^{-1}	C_4^{-1}	e	C_4	C_4^2	σ_{d_2}	σ_{d_1}	σ_x	σ_y
σ_x	σ_x	σ_{d_2}	σ_y	σ_{d_1}	e	C_4^2	C_4^{-1}	C_4
σ_y	σ_y	σ_{d_1}	σ_x	σ_{d_2}	C_4^2	e	C_4	C_4^{-1}
σ_{d_1}	σ_{d_1}	σ_x	σ_{d_2}	σ_y	C_4	C_4^{-1}	e	C_4^2
σ_{d_2}	σ_{d_2}	σ_y	σ_{d_1}	σ_x	C_4^{-1}	C_4	C_4^2	e

Table 4.1: Group multiplication table of the group C_{4v}.

and $2\sigma_v = \{\sigma_x, \sigma_y\}$. The character $\chi^\Gamma(g)$ of a representation Γ is the trace of the representation matrix $D^\Gamma(g)$ of a certain group element g. Since the trace is cyclic, then for conjugate group elements A and B

$$
\begin{aligned}
\chi^\Gamma(B) &= \mathrm{Tr}\left(D^\Gamma(g)D^\Gamma(A)D^\Gamma(g^{-1})\right) \\
&= \mathrm{Tr}\left(D^\Gamma(g^{-1})D^\Gamma(g)D^\Gamma(A)\right) \\
&= \mathrm{Tr}\left(D^\Gamma(g^{-1}g)D^\Gamma(A)\right) = \chi^\Gamma(A).
\end{aligned}
\tag{4.41}
$$

This means that the representation of all group elements in a certain conjugation class has the same character.

It is useful to list the characters of the different conjugation classes in a table of the different irreducible representations of a group. This is because the number of conjugation classes of a finite group is the same as the number of irreducible representations of that group. This table is known as the character table of the group. The character table of the group C_{4v} is shown in Table 4.2. This table can be derived without knowing the details of the irreducible representations but in stead using character relations from basic group theory.[2]

The dimensionality of the irrep. can be found in Table 4.2 by looking up the first column, i.e. the column giving the character of the conjugation class $\{e\}$. Since the group element e maps to the identity transformation in all representations then its trace gives the dimension of the representation. From the table we see that all the irreducible representations are 1-dimensional except for Γ_5 which is 2 dimensional. All

---

2. Many of these relations are derived from the great orthogonality theorem which can be found e.g. in [2].

C_{4v}	e	$2C_4$	C_4^2	$2\sigma_v$	$2\sigma_d$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1
Γ_5	2	0	-2	0	0

Table 4.2: Character table of the group C_{4v}.

the 1-dimensional irreducible representation matrices are then completely determined by the character table since they are just given by the characters themselves, i.e. $D^{\Gamma_2}(\sigma_x) = -1$.

To find a 2-dimensional representation of C_{4v} we can imagine how a normal 2D vector $(x, y)^\mathsf{T} \in \mathbb{R}^2$ behaves under its transformations. We take again the example of a counter clockwise rotation by 90° which tranforms a vector

$$C_4 : \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ x \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{4.42}$$

Obviously, the matrix

$$D^{(\Gamma_5)}(C_4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4.43}$$

is the representation matrix of a two-dimensional representation of C_4. Continuing in this way for all the group tranformations yields the matrices

$$D^{(\Gamma_5)}(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad D^{(\Gamma_5)}(C_4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4.44a}$$

$$D^{(\Gamma_5)}(C_4^{-1}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad D^{(\Gamma_5)}(C_4^2) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.44b}$$

$$D^{(\Gamma_5)}(\sigma_x) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad D^{(\Gamma_5)}(\sigma_y) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.44c}$$

$$D^{(\Gamma_5)}(\sigma_{d_1}) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \qquad D^{(\Gamma_5)}(\sigma_{d_2}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.44d}$$

4.8 Square Lattice Harmonics

Since $\psi(\boldsymbol{k})$ and $\boldsymbol{d_k}$ are invariant with respect to translation by any resiprocal lattice vector $\boldsymbol{Q}$: $\psi(\boldsymbol{k} + \boldsymbol{Q}) = \psi(\boldsymbol{k})$, they can be expanded in

a discrete Fourier transform over the real lattice, such that

$$\psi(\boldsymbol{k}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \cos \boldsymbol{R} \cdot \boldsymbol{k}, \qquad (4.45)$$

and

$$\boldsymbol{d_k} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \boldsymbol{d_R} \sin \boldsymbol{R} \cdot \boldsymbol{k}, \qquad (4.46)$$

where the exponential of the Fourier transform has been reduced to trigonometric functions by the parity of the functions.

We are interested in the basis vectors $|\Gamma, q, m\rangle$ of the representations of the symmetry group C_{4v} of the $2D$ square lattice. In this ket notation, Γ gives the irrep. , m enumerates the basis vectors in case the irrep. is multi-dimensional, while q gives the version of the irrep. in case the space of possible $|v\rangle$ permits multiple versions of the same irrep. In the active view of group transformations, the question of finding the basis vectors translates to finding the basis functions of the functions $\psi(\boldsymbol{k})$ and $\boldsymbol{d_k}$. In Section 4.4.3 we saw how these functions transformed under group transformations. In Section 4.4.4 we saw how the projection operators could be used to extract individual basis vectors. We will now use these operators on the Fourier expansions of $\psi(\boldsymbol{k})$ and $\boldsymbol{d_k}$ to extract possible basis functions given the symmetry group of the square lattice.

4.8.1 Even basis functions

4.9 Decomposition of the Potential

Let at first $\hat{V}$ be a general two-body operator that acts on an N-particle state which is a vector in $\mathcal{H}_N = \otimes_{i=1}^{N} \mathcal{H}$. The single particle Hilbert space $\mathcal{H}$ in question is quantified by momentum and spin such that $\mathcal{H} = \text{span}\{|\boldsymbol{k}, s\rangle\}$. Denoting specific combinations of $\boldsymbol{k}$ and s as α as a shorthand for the moment, then $\hat{V}$ acts on basis vectors in $\mathcal{H}_N$ as

$$\hat{V}|\alpha_1\rangle \ldots |\alpha_N\rangle = \sum_{1 \leq i < j \leq N} \hat{V}_{ij}|\alpha_1\rangle \ldots |\alpha_N\rangle, \qquad (4.47)$$

by definition of being a two-body operator. Here $\hat{V}_{ij}$ is an operator that only acts on the ith and jth ket. Even though $\hat{V}$ acts on $\mathcal{H}_N$, because of how it can be written in terms of $\hat{V}_{ij}$ and this only acts on two states

at a time, it follows that $\hat{V}$ is completely determined by its action on the reduced Hilbert space $\mathcal{H}_2$. This implies that $\hat{V}$ is fully described by its matrix elements

$$\langle \alpha | \langle \alpha' | \hat{V} | \beta \rangle | \beta' \rangle. \tag{4.48}$$

Inserting back the $|\boldsymbol{k}, s\rangle$ notation, these matrix elements are referred to as

$$V_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \boldsymbol{k}_4;\, s_1 s_2 s_3 s_4} = \langle \boldsymbol{k}_1 s_1 | \langle \boldsymbol{k}_2 s_2 | \hat{V} | \boldsymbol{k}_4 s_4 \rangle | \boldsymbol{k}_3 s_3 \rangle. \tag{4.49}$$

When $\hat{V}$ is a BCS operator acting on the BCS Hilbert space described in the previous section, these matrix elements are denoted

$$V_{\boldsymbol{k}\boldsymbol{k}';\, s_1 s_2 s_3 s_4} = \langle \boldsymbol{k}s_1 | \langle -\boldsymbol{k}s_2 | \hat{V} | \boldsymbol{k}' s_4 \rangle | -\boldsymbol{k}' s_3 \rangle. \tag{4.50}$$

Since $\hat{V}$ is Hermitian, it must be diagonalizable in a basis of eigenfunctions. Barring accidental degeneracy, a basis for a d-degenerate eigenvalue is also a basis for an irreducible representation of the symmetry group G of the Hamiltonian. In the case of accidental degeneracy then this d-dimensional vector space consists of several non-intersecting subspaces where each subspace is a basis for a (possibly different) irrep. Note that this does not mean that (barring accidental degeneracy) there exists one seperate eigenvalue for each irrep. of G since there might be several different eigenvalues with different eigenspace bases but where all of them are bases for the same irrep. Regardless of these details, the connection between irreducible representations and the eigenvalues of $\hat{V}$ is a great help in finding the bases for which it is diagonal.

We let the basis for a d_Γ-dimensional irrep. Γ be denoted $\{|\Gamma, q_\Gamma, m\rangle\}_{m=1}^{d_\Gamma}$, where $\hat{V}$ has an eigenvalue V_{Γ, q_Γ} for the vectors in this basis and q_Γ is an index enumerating the different versions of bases of Γ that $\hat{V}$ might have in its set of eigenspace bases. Since $\hat{V}$ then is diagonal in this set of bases then

$$\hat{V} = \sum_{\Gamma q_\Gamma} V_{\Gamma, q_\Gamma} \sum_{m=1}^{d_\Gamma} |\Gamma, q_\Gamma, m\rangle \langle \Gamma, q_\Gamma, m|. \tag{4.51}$$

Because of the potential for accidental degeneracy we can not guarantee that $V_{\Gamma, q_\Gamma} \neq V_{\Gamma', q_{\Gamma'}}$ for different Γ and Γ'. Inserting this expression for $\hat{V}$ into the matrix elements in Eq. (4.50) lets us write them

in terms of irreducible representation basis vectors in the momentum spin function representation:

$$V_{\boldsymbol{k}\boldsymbol{k}';\,s_1 s_2 s_3 s_4} = \sum_\Gamma V_{\Gamma,q_\Gamma} \sum_{m=1}^{d_\Gamma} \Psi_{s_1 s_2}^{\Gamma,q_\Gamma}(\boldsymbol{k})\Psi_{s_3 s_4}^{\Gamma,q_\Gamma}(-\boldsymbol{k}')^\dagger, \qquad (4.52)$$

where

$$\Psi_{s_1 s_2}^{\Gamma,q_\Gamma}(\boldsymbol{k}) = \langle \boldsymbol{k}, s_1 | \langle -\boldsymbol{k}, s_2 \mid \Gamma, q_\Gamma, m \rangle. \qquad (4.53)$$

We can separate the set of different irreducible representation bases into bases that have vectors that transform either symmetrically or anti-symmetrically with respect to the group element of space inversion P. We call the representations of such bases even or odd representations. Even representations are those that map P to the identity operator $\mathbb{1}$ and as a consequence have $\Psi_{s_1 s_2}^{\Gamma,q_\Gamma,m}(-\boldsymbol{k}) = \Psi_{s_1 s_2}^{\Gamma,q_\Gamma,m}(\boldsymbol{k})$. Writing the spin-indices in these functions in terms of Pauli matrices by using the expansion in Eq. (4.9) and using the fermionic symmetry then even representations a have

$$\Psi_{s_1 s_2}^{a,q_a,m}(\boldsymbol{k}) = \psi_{\boldsymbol{k}}^{a,q_a,m} i\sigma_{s_1 s_2}^{y}. \qquad (4.54)$$

Odd representations b map P to the inversion operator I such that $\Psi_{s_1 s_2}^{b,q_b,m}(-\boldsymbol{k}) = -\Psi_{s_1 s_2}^{b,q_b,m}(\boldsymbol{k})$. Expanding in Pauli matrices then yields

$$\Psi_{s_1 s_2}^{b,q_b,m}(\boldsymbol{k}) = \boldsymbol{d}_{\boldsymbol{k}}^{b,q_b,m} \cdot (\boldsymbol{\sigma} i\sigma^y)_{s_1 s_2}. \qquad (4.55)$$

Separating the sum over irreducible representations Γ into sums over even (a) and odd (b) representations in the potential operator matrix elements in Eq. (4.52), we arrive at the fully expanded expression

$$V_{\boldsymbol{k}\boldsymbol{k}';\,s_1 s_2 s_3 s_4} = \sum_{a q_a} V_{a,q_a} \sum_{m=1}^{d_a} \psi_{\boldsymbol{k}}^{a,q_a,m} i\sigma_{s_1 s_2}^{y} \left(\psi_{-\boldsymbol{k}'}^{a,q_a,m} i\sigma_{s_3 s_4}^{y}\right)^\dagger$$

$$+ \sum_{b q_b} V_{b,q_b} \sum_{m=1}^{d_b} (\boldsymbol{d}_{\boldsymbol{k}}^{b,q_b,m} \cdot \boldsymbol{\sigma} i\sigma^y)_{s_1 s_2} \left[(\boldsymbol{d}_{-\boldsymbol{k}'}^{b,q_b,m} \cdot \boldsymbol{\sigma} i\sigma^y)_{s_3 s_4}\right]^\dagger.$$
$$(4.56)$$

In this use of the dagger notation, the adjoint acts on both of the matrix indices such that $\boldsymbol{d}_{-\boldsymbol{k}}^\dagger = \boldsymbol{d}_{\boldsymbol{k}}^*$ and $\sigma_{s_1 s_2}^\dagger = \sigma_{s_2 s_1}^*$.

CHAPTER 5

Lattice Models

When we have a model for the free energy of a statistical mechanical system that is too complicated to calculate analytically one approach is to utilize computers and Monte-Carlo techniques. To make numerical methods more effective one common approach is to discretize continuous models down on a discrete numerical lattice. The lattice can in principle be of any form as long as the continuum limit reproduces the original theory, however in this thesis we will exclusively focus on a square numerical lattice due to its simple form.

In this chapter we will introduce different aspects of discretizing a continuous free-energy model down on a square numerical lattice.

5.1 Discretizing derivatives

5.2 Boundary Conditions

5.3 Including an external field

5.3.1 Symmetric Landau gauge

Monte-Carlo Techniques

In this chapter we discuss some techniques useful in Monte-Carlo simulations of systems in statistical-physics.

6.1 Metropolis-Hastings method

6.2 Importance sampling of observables

6.3 Thermalization procedures

6.4 Parallell tempering

6.5 Reweighting

CHAPTER 7

Vortices in superconductors

7.1 Vorticity observables

7.2 Double quanta vorticies

7.3 Vortex lattices

7.4 Vortex lattice transitions

Example chapter

This chapter serves as a simple demonstration of what the thesis template looks like. It provides some simple examples of typical content in academic theses; see e.g. table 8.1, figure 8.1, and equation (8.2). In addition, it shows what the default chapters, sections, and margins look like. For completeness, we also include some references [3–5].

8.1 Here is an example section

Here is an example of a display equation: a self-consistency equation taken from the study of superconductivity. Note that all equations are left-justified instead of centered. In text with a large number of short display equations, this makes the text easier to follow with your eyes, since they don't have to jump large distances at a time. It also makes the page look more organized due to the constant indentation level.

$$\Delta(z) = \int_0^\infty d\epsilon \ \mathrm{Re}[f_s(\epsilon)] \tanh\left(\frac{\pi}{2e^\gamma}\frac{\epsilon/\Delta_0}{T/T_c}\right) \tag{8.1}$$

Here is another example, in the form of Maxwell's equations. Note the consistent indentation level compared to the equation above.

$$\begin{aligned}\nabla \cdot \mathbf{D} = \rho, \quad &\nabla \times \mathbf{E} = 0 - \partial_t \mathbf{B}; \\ \nabla \cdot \mathbf{B} = 0, \quad &\nabla \times \mathbf{H} = \mathbf{J} + \partial_t \mathbf{D}.\end{aligned} \tag{8.2}$$

Finally, we will show some examples of tables and figures. Note how the width of table 8.1 matches the indentation level of the equations.
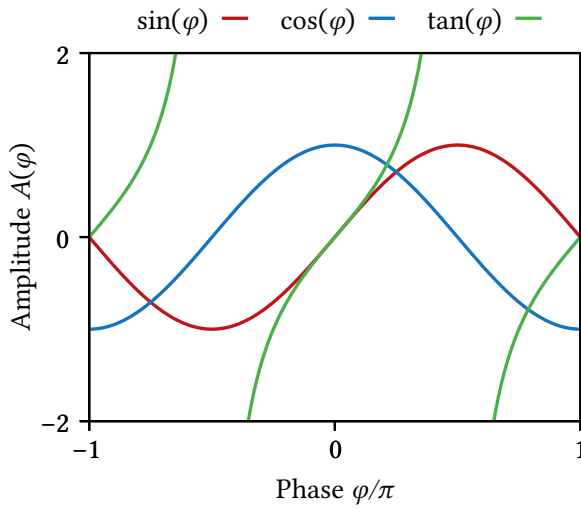
Figure 8.1: This is an example figure made by GNUPLOT. I have also included an intentionally long caption to show the margins.

The captions are formatted using a small font and extra margins, which helps separate the captions from the surrounding text.

8.2 Lorem ipsum

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus

Table 8.1: Test table with some mathematical constants.

Name	Symbol	Value
Euler constant	e	$2.71\ldots$
Circle constant	π	$3.14\ldots$
Imaginary identity	i	$\sqrt{-1}$

vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagit-

tis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetuer.

Suspendisse vel felis. Ut lorem lorem, interdum eu, tincidunt sit amet, laoreet vitae, arcu. Aenean faucibus pede eu ante. Praesent enim elit, rutrum at, molestie non, nonummy vel, nisl. Ut lectus eros, malesuada sit amet, fermentum eu, sodales cursus, magna. Donec eu purus. Quisque vehicula, urna sed ultricies auctor, pede lorem egestas dui, et convallis elit erat sed nulla. Donec luctus. Curabitur et nunc. Aliquam dolor odio, commodo pretium, ultricies non, pharetra in, velit. Integer arcu est, nonummy in, fermentum faucibus, egestas vel, odio.

Sed commodo posuere pede. Mauris ut est. Ut quis purus. Sed ac odio. Sed vehicula hendrerit sem. Duis non odio. Morbi ut dui. Sed accumsan risus eget odio. In hac habitasse platea dictumst. Pellentesque non elit. Fusce sed justo eu urna porta tincidunt. Mauris felis odio, sollicitudin sed, volutpat a, ornare ac, erat. Morbi quis dolor. Donec pellentesque, erat ac sagittis semper, nunc dui lobortis purus, quis congue purus metus ultricies tellus. Proin et quam. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Praesent sapien turpis, fermentum vel, eleifend faucibus, vehicula eu, lacus.

CHAPTER 9

Conclusion

This would be a natural place to summarize your main results, and perhaps provide an outlook for future developments in the field.

Bibliography

1. **H.K. Onnes.**
    The disappearance of the resistivity of mercury.
    Commun. Phys. Lab. Univ. Leiden (May 1911).

2. **T. Inui, Y. Tanabe, Y. Onodera.**
    Group Theory and Its Applications in Physics (1990).
    DOI: 10.1007/978-3-642-80021-4

3. **R. Feynman, R. Leighton, M. Sands.**
    The Feynman Lectures on Physics 2nd edition, 36–38 (1963).
    ISBN: 9780201021165

4. **M. Lipovaca.**
    Learn You a Haskell for Great Good! 1st ed. (2011).
    ISBN: 9781593272838

5. **J. Beringer** *et al.*
    Review of Particle Physics.
    Physical Review D 86, 10–20 (2012).
    DOI: 10.1103/physrevd.86.010001