

# Abstract

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## **Preface**

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



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## 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 superior 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 precisely 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  $-268.99^{\circ}\text{C}$  and then Dr. Onnes measured the resistivity, which is a measure of how much energy is used to push electrons through a ma-

material. He found that the resistivity suddenly disappeared at this temperature and lower. It was expected that the resistivity would become lower with temperature but the extreme suddenness of the disappearance was surprising. Not only did resistivity disappear 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  $-268.99^{\circ}\text{C}$ . 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.

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## 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 ensemble 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 ensemble can then be written

$$Z = \sum_i e^{-\beta E_i}, \quad (2.1)$$

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

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<sup>1</sup>

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

## 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 ensemble. 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 calculate 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,

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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  $dr dp$  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 observable is

$$\langle O \rangle = \sum_j o_j P_j. \quad (2.3)$$

The probability distribution  $P_j$  is given by

$$P_j = e^{-\beta E_j} / Z, \quad (2.4)$$

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

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

## 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-Landau theory of superconductivity is based on Landau's previous work on a theory for general second order phase-transitions<sup>2</sup>

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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 appearance of some kind of measurable order that can be described by a function  $\psi$  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,<sup>3</sup> 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<sup>4</sup> can be expanded in a Maclaurin-series with respect to this parameter as

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

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  $\psi$  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  $\Psi$  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  $\Psi$  is complex it has to be combined with its complex conjugate  $\Psi^*$  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

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3. The astute reader might have noticed that this example is a first order phase transition because of the existence 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

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

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

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

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.<sup>5</sup>

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  $\Psi$  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

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

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

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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

$$F = \int d^3r f(\Psi, \nabla\Psi, \nabla^2\Psi, \nabla^3\Psi, \dots). \quad (2.10)$$

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  $\mathbf{A}$  times a constant is subtracted with from any momentum in the previously neutral theory. Specifically  $\mathbf{p} \mapsto \mathbf{p} - q/c\mathbf{A}$  where  $q$  is the charge of the particle and  $c$  is the speed of light.

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

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## 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  $\Gamma_{5u}^-$  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  $D(g): V \rightarrow V$ . Then a subspace  $U \subseteq V$  is *invariant* if

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

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

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

### 4.2.1 Application of group elements

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. A basis for this space is given by the vectors  $|\mathbf{k}, s\rangle$  in the Dirac notation. Given  $\mathbf{k} \in \mathbb{R}^d$  and  $s \in \{\uparrow, \downarrow\}$ , these basis vectors transform according to

$$g : |\mathbf{k}', s'\rangle = \sum_{\mathbf{k}s} |\mathbf{k}, s\rangle D_{g \, ss'} \delta_{\mathbf{k}, g\mathbf{k}'}, \quad (4.3)$$

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  $\mathbb{R}^d$ , and  $D_{g \, ss'}$  is the  $SU(2)$  representation.

### 4.2.2 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  $b_m^{(\alpha)}$  where  $m$  thus counts the number of basis vectors in each irrep. Then an arbitrary vector  $f \in V$  can be written in terms of these basis vectors as

$$f = \sum_{\alpha} \sum_m c_m^{(\alpha)} b_m^{(\alpha)}. \quad (4.4)$$

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

$$P_{lm}^{(\beta)} f = c_m^{(\beta)} b_l^{(\beta)}. \quad (4.5)$$

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

$$P_{l,m}^{(\beta)} = \frac{d_{\beta}}{|G|} \sum_{g \in G} D_{lm}^{(\beta)}(g)^* g :, \quad (4.6)$$

where  $d_{\beta}$  is the dimension of irrep.  $\beta$ ,  $D_{lm}^{(\beta)}(g)$  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  $b_m^{(\alpha)}$ . Since the relevant representation of  $g$  in this case is the irreducible representation for which  $b_m^{(\alpha)}$  is a basis vector, the application becomes

$$g : b_m^{(\alpha)} = \sum_n b_n^{(\alpha)} D_{nm}^{(\alpha)}(g). \quad (4.7)$$

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

$$P^{(\beta)} \equiv \sum_l P_l^{(\beta)} = \frac{d_{\beta}}{|G|} \sum_{g \in G} \sum_l D_{ll}^{(\beta)}(g)^* g := \frac{d_{\beta}}{|G|} \sum_{g \in G} \chi^{(\beta)}(g)^* g :. \quad (4.8)$$

### 4.2.3 Representation on product spaces

## 4.3 Fermionic symmetry transformations

### 4.4 Time-reversal symmetry

## 4.5 Square Lattice Harmonics

## 4.6 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  $\mathcal{H} = \text{span}\{|\mathbf{k}, s\rangle\}$  and we only consider states that have opposite momentum. Thus this Hilbert space is given by

$$\mathcal{B} = \text{span}\{|\mathbf{k}, s_1\rangle|-\mathbf{k}, s_2\rangle\}, \quad (4.9)$$

and the identity operator in this space can be written

$$\hat{\mathbb{1}} = \sum_{\mathbf{k} s_1 s_2} |\mathbf{k}, s_1\rangle|-\mathbf{k}, s_2\rangle\langle-\mathbf{k}, s_2|\langle\mathbf{k}, s_1|. \quad (4.10)$$

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

$$|v\rangle = \sum_{\mathbf{k} s_1 s_2} v_{s_1 s_2}(\mathbf{k}) |\mathbf{k}, s_1\rangle|-\mathbf{k}, s_2\rangle, \quad (4.11)$$

where

$$v_{s_1 s_2}(\mathbf{k}) = \langle-\mathbf{k}, s_2|\langle\mathbf{k}, s_1|v\rangle. \quad (4.12)$$

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  $v_{s_1 s_2}(\mathbf{k})$ . Putting these different realizations of  $v_{s_1 s_2}(\mathbf{k})$  as elements in a  $2 \times 2$  matrix we get

$$v_{s_1 s_2}(\mathbf{k}) = \begin{pmatrix} v_{\uparrow\uparrow}(\mathbf{k}) & v_{\uparrow\downarrow}(\mathbf{k}) \\ v_{\downarrow\uparrow}(\mathbf{k}) & v_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix}. \quad (4.13)$$

Any  $2 \times 2$  matrix can be written in the conventional basis of the 4 Pauli matrices  $\sigma^0 = \mathbb{1}_{2 \times 2}$ ,  $\sigma^x$ ,  $\sigma^y$ , and  $\sigma^z$ . This means that we could write the matrix in Eq. (4.13)

$$v_{s_1 s_2}(\mathbf{k}) = v_{\mathbf{k}}^0 \sigma_{s_1 s_2}^0 + v_{\mathbf{k}}^i \sigma_{s_1 s_2}^i. \quad (4.14)$$

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  $\mathbf{k}$  that is in front of  $\sigma^0$  be called  $\psi_{\mathbf{k}}$ . The three others are conventionally denoted  $d_{\mathbf{k},i}$ . Expanded in this conventional basis then  $v_{s_1 s_2}(\mathbf{k})$  takes the form

$$v_{s_1 s_2}(\mathbf{k}) = (\psi_{\mathbf{k}} \sigma_{s_1 s'}^0 + d_{\mathbf{k},i} \sigma_{s_1 s'}^i) i \sigma_{s' s_2}^y, \quad (4.15)$$

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

$$|v\rangle = \sum_{\mathbf{k} s_1 s_2} [(\psi_{\mathbf{k}} \sigma^0 + \mathbf{d}_{\mathbf{k}} \cdot \boldsymbol{\sigma}) i \sigma^y]_{s_1 s_2} |\mathbf{k}, s_1\rangle |-\mathbf{k}, s_2\rangle. \quad (4.16)$$

Going one step back and writing out the different combinations of  $s_1 s_2$  in  $v_{s_1 s_2}(\mathbf{k})$  as a matrix like we did in Eq. (4.13), but now multiplying out the Pauli matrices in Eq. (4.15) we get

$$\begin{pmatrix} v_{\uparrow\uparrow}(\mathbf{k}) & v_{\uparrow\downarrow}(\mathbf{k}) \\ v_{\downarrow\uparrow}(\mathbf{k}) & v_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_{\mathbf{k},x} + i d_{\mathbf{k},y} & \psi_{\mathbf{k}} + d_{\mathbf{k},z} \\ -\psi_{\mathbf{k}} + d_{\mathbf{k},z} & d_{\mathbf{k},x} + i d_{\mathbf{k},y} \end{pmatrix}. \quad (4.17)$$

This set of linear relations is easily inverted to yield

$$\psi_{\mathbf{k}} = \frac{1}{2}(v_{\uparrow\downarrow}(\mathbf{k}) - v_{\downarrow\uparrow}(\mathbf{k})) \quad (4.18)$$

$$d_{\mathbf{k},x} = \frac{1}{2}(v_{\downarrow\downarrow}(\mathbf{k}) - v_{\uparrow\uparrow}(\mathbf{k})) \quad (4.19)$$

$$d_{\mathbf{k},y} = -\frac{i}{2}(v_{\uparrow\uparrow}(\mathbf{k}) + v_{\downarrow\downarrow}(\mathbf{k})) \quad (4.20)$$

$$d_{\mathbf{k},z} = \frac{1}{2}(v_{\uparrow\downarrow}(\mathbf{k}) + v_{\downarrow\uparrow}(\mathbf{k})). \quad (4.21)$$

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

$$|\mathbf{k}, s_1\rangle |-\mathbf{k}, s_2\rangle = -|-\mathbf{k}, s_2\rangle |\mathbf{k}, s_1\rangle. \quad (4.22)$$

Using this symmetry transformation on the basis vectors in the expansion of  $|v\rangle$  in Eq. (4.12), then renaming indices and finally equating coefficients term by term, we see that for the coefficients of  $|v\rangle$ , this symmetry takes the form

$$v_{s_1 s_2}(\mathbf{k}) = -v_{s_2 s_1}(-\mathbf{k}). \quad (4.23)$$

## 4.7 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  $\mathcal{H} = \text{span}\{|\mathbf{k}, s\rangle\}$ . Denoting specific combinations of  $\mathbf{k}$  and  $s$  as  $\alpha$  as a shorthand for the moment, then  $\hat{V}$  acts on basis vectors in  $\mathcal{H}_N$  as

$$\hat{V}|\alpha_1\rangle \dots |\alpha_N\rangle = \sum_{1 \leq i < j \leq N} \hat{V}_{ij}|\alpha_1\rangle \dots |\alpha_N\rangle, \quad (4.24)$$

by definition of being a two-body operator. Here  $\hat{V}_{ij}$  is an operator that only acts on the  $i$ th and  $j$ th 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

$$\langle \alpha | \langle \alpha' | \hat{V} | \beta \rangle | \beta' \rangle. \quad (4.25)$$

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

$$V_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4; s_1 s_2 s_3 s_4} = \langle \mathbf{k}_1 s_1 | \langle \mathbf{k}_2 s_2 | \hat{V} | \mathbf{k}_4 s_4 \rangle | \mathbf{k}_3 s_3 \rangle. \quad (4.26)$$

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

$$V_{\mathbf{k} \mathbf{k}'; s_1 s_2 s_3 s_4} = \langle \mathbf{k} s_1 | \langle -\mathbf{k} s_2 | \hat{V} | \mathbf{k}' s_4 \rangle | -\mathbf{k}' s_3 \rangle. \quad (4.27)$$

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 different irrep. Note that this does not mean that (barring accidental degeneracy) there exists one separate 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, this 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  $d_\Gamma$ -dimensional irrep.  $\Gamma$  be denoted  $\{|\Gamma, q_\Gamma, m\rangle\}_{m=1}^{d_\Gamma}$ , where  $\hat{V}$  has an eigenvalue  $V_{\Gamma, q_\Gamma}$  for the vectors in this basis and  $q_\Gamma$  is an index enumerating the different versions of bases of  $\Gamma$  that  $\hat{V}$  might have in its set of eigenspace bases. Since  $\hat{V}$  then is in this set of bases then

$$\hat{V} = \sum_{\Gamma, q_\Gamma} V_{\Gamma, q_\Gamma} \sum_{m=1}^{d_\Gamma} |\Gamma, q_\Gamma, m\rangle \langle \Gamma, q_\Gamma, m|. \quad (4.28)$$

Because of the potential for accidental degeneracy we can not guarantee that  $V_{\Gamma, q_\Gamma} \neq V_{\Gamma', q_{\Gamma'}}$  for different  $\Gamma$  and  $\Gamma'$ . Inserting this expression for  $\hat{V}$  into the matrix elements in Eq. (4.27) lets us write them in terms of irreducible representation basis vectors in the momentum spin function representation:

$$V_{\mathbf{k}\mathbf{k}'; s_1 s_2 s_3 s_4} = \sum_{\Gamma} V_{\Gamma, q_\Gamma} \sum_{m=1}^{d_\Gamma} \Psi_{s_1 s_2}^{\Gamma, q_\Gamma}(\mathbf{k}) \Psi_{s_3 s_4}^{\Gamma, q_\Gamma}(-\mathbf{k}')^\dagger, \quad (4.29)$$

where

$$\Psi_{s_1 s_2}^{\Gamma, q_\Gamma}(\mathbf{k}) = \langle \mathbf{k}, s_1 | \langle -\mathbf{k}, s_2 | \Gamma, q_\Gamma, m \rangle. \quad (4.30)$$

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  $\Psi_{s_1 s_2}^{\Gamma, q_\Gamma, m}(-\mathbf{k}) = \Psi_{s_1 s_2}^{\Gamma, q_\Gamma, m}(\mathbf{k})$ . Writing the spin-indices in these functions in terms of Pauli matrices by using the expansion in Eq. (4.15) and using the fermionic symmetry then even representations  $a$  have

$$\Psi_{s_1 s_2}^{a, q_a, m}(\mathbf{k}) = \psi_{\mathbf{k}}^{a, q_a, m} i\sigma_{s_1 s_2}^y. \quad (4.31)$$

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

$$\Psi_{s_1 s_2}^{b, q_b, m}(\mathbf{k}) = \mathbf{d}_{\mathbf{k}}^{b, q_b, m} \cdot (\boldsymbol{\sigma} i\sigma^y)_{s_1 s_2}. \quad (4.32)$$

Separating the sum over irreducible representations  $\Gamma$  into sums over even ( $a$ ) and odd ( $b$ ) representations in the potential operator matrix

elements in Eq. (4.29), we arrive at the fully expanded expression

$$\begin{aligned}
V_{\mathbf{k}\mathbf{k}'; s_1 s_2 s_3 s_4} &= \sum_{a q_a} V_{a, q_a} \sum_{m=1}^{d_a} \psi_{\mathbf{k}}^{a, q_a, m} i \sigma_{s_1 s_2}^y (\psi_{-\mathbf{k}'}^{a, q_a, m} i \sigma_{s_3 s_4}^y)^\dagger \\
&+ \sum_{b q_b} V_{b, q_b} \sum_{m=1}^{d_b} (d_{\mathbf{k}}^{b, q_b, m} \cdot \boldsymbol{\sigma} i \sigma^y)_{s_1 s_2} \left[ (d_{-\mathbf{k}'}^{b, q_b, m} \cdot \boldsymbol{\sigma} i \sigma^y)_{s_3 s_4} \right]^\dagger.
\end{aligned} \tag{4.33}$$



## 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



# CHAPTER 6

## 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 Parallel tempering

### 6.5 Reweighting



## **Vortices in superconductors**

### **7.1 Vorticity observables**

### **7.2 Double quanta vortices**

### **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 [2–4].

### 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.

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

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

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

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.

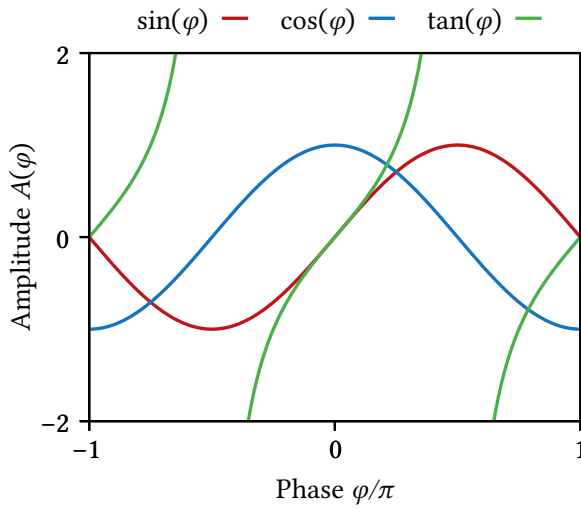


Figure 8.1: This is an example figure made by `GNUPLOT`. I have also included an intentionally long caption to show the margins.

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

## 8.2 Lorem ipsum

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Table 8.1: Test table with some mathematical constants.

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



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# 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.



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