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 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 $-268.99\,°C$ 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 ensamble 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

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

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 implicitely 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,

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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 $\mathrm{d}r\,\mathrm{d}p$ 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]

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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 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

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

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

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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

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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

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

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.

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

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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.

A field theoretic expression for the quantum mechanical partition function $\mathcal{Z}$ is obtained by using a coherent state basis. A coherent state is the eigen-state of an annihilation operator, thus it produces an eigenvalue when operated on by the annihilation operator. Letting $\hat{H}$ be the quantum mechanical Hamiltonian of the system for which we are interested in calculating the parition function, μ the the chemical potential and $\hat{N}$ is the number operator then the partition function

$$\mathcal{Z} = \text{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})}). \tag{3.1}$$

Inserting a basis of coherent states $\{|\xi\rangle\}$ when calculating the trace, we obtain a functional integral over the coherent state eigenvalues ξ_α and ξ_α^* which substitute the annihilation and creation operators c_α and $c_\alpha^\dagger$ respectively. Here α symbolize the collection of quantum-numbers needed to specify a state. The functional integral then takes the form

$$\mathcal{Z} = \int \mathcal{D}[\xi^*\,\xi]e^{-\int_0^\beta d\tau \sum_\alpha [\xi_\alpha^*(\partial_\tau-\mu)\xi_\alpha+H(\xi_\alpha,\xi_\alpha^*)]}. \tag{3.2}$$

The integration variable τ is the imaginary time and a τ dependence is implicit in the notation such that $\xi_\alpha = \xi_\alpha(\tau)$. This path-integral no-

tation is a shorthand for a more involved expression where the imaginary time-dependence of τ is split into a collection of time-indexed coherent state eigenfunctions $\xi_{\alpha,\tau}$ and the integration measure is a product over these indices and the quantum-state indices α. For further detail we refer to Ref. [2] which we will follow for a large part of this chapter.

3.1 Quadratic Fermionic Field Integrals

Because of the anti-commuting property of the fermion annihilation operators, any coherent state[1] has to have eigenvalues that anti-commute as well. This leads to the partition function written in the convenient basis of the coherent states being constructed with Graßmann numbers as the central variables.

3.1.1 Graßmann algebras

A Graßmann algebra is constructed on a set of generators $\{\xi_\alpha\}$ such that a specific product of the generators $\xi_{\alpha_1}\xi_{\alpha_2}\cdots\xi_{\alpha_n}$ together with a complex coefficient ϕ constitute a number in the algebra and the generators anti-commute such that $\xi_\alpha\xi_\beta = -\xi_\beta\xi_\alpha$. On such an algebra, differentiation can be defined such that

$$\frac{\mathrm{d}}{\mathrm{d}\xi_{\alpha_m}}\,\phi\,\xi_{\alpha_1}\cdots\xi_{\alpha_n} = (-1)^m\phi\,\xi_{\alpha_1}\cdots\xi_{\alpha_{m-1}}\xi_{\alpha_{m+1}}\cdots\xi_{\alpha_n}, \qquad (3.3)$$

provided the generator ξ_{α_m} is in the number and 0 otherwise. The factors of (-1) comes from anti-commuting the generator ξ_{α_m} such that it is next to the differentiation operator. In Graßmann algebra, integration can be (perhaps a little non-intuitively) be defined such that it acts in the same way as differentiation, i.e. generators have to be anti-commuted until they are next to the symbolic differential symbol $\mathrm{d}\xi_\alpha$, and then

$$\int \mathrm{d}\xi\,\xi = 1, \qquad (3.4)$$

while

$$\int \mathrm{d}\xi\,1 = 0. \qquad (3.5)$$

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1. An eigenstate of the annihilation operator

On an algebra consisting of $2n$ generators we define conjugation as a map from the first half of the generators $\{\xi_{\alpha_i}\}_{i=1}^n$ to the other half $\{\xi_{\alpha_i}^*\}_{i=1}^n$ and in such a way that when applied to a particular number

$$(\phi \xi_\alpha \xi_\beta)^* = \phi^* \xi_\beta^* \xi_\alpha^*. \tag{3.6}$$

3.1.2 Nambu Spinor

In the Nambu notation we group spin-dependent Graßmann numbers $\xi_\uparrow$ and $\xi_\downarrow^*$, which correspond to the annihilation- and creation-operators $\hat{c}_\uparrow^\dagger$ and $\hat{c}_\downarrow$, in a vector called a Nambu spinor

$$\boldsymbol{\xi} = \begin{pmatrix} \xi_\uparrow \\ \xi_\downarrow^* \end{pmatrix}. \tag{3.7}$$

A sesquilinear form can then be created with this vector and its adjoint such that

$$\boldsymbol{\xi}^\dagger S \boldsymbol{\xi} = S_{11} \xi_\uparrow^* \xi_\uparrow + S_{22} \xi_\downarrow^* \xi_\downarrow + S_{12} \xi_\uparrow^* \xi_\downarrow^* + S_{21} \xi_\uparrow \xi_\downarrow. \tag{3.8}$$

This allows any action that contains spin-dependent terms of the form of the right hand side of Eq. (3.8) to be put on sesquilinear form. Assuming this is the case, then the partition function in the field-integral representation takes the form

$$\mathcal{Z} = \int \mathcal{D}[\xi^* \, \xi] \; e^{- \int_0^\beta \mathrm{d}\tau \, \boldsymbol{\xi}_\gamma^\dagger S_{\gamma\delta} \boldsymbol{\xi}_\delta}. \tag{3.9}$$

In this equation, the indices γ and δ is an arbitrary collection of quantum numbers needed to specify a state other than spin, for example they could be momentum indices $\gamma = \boldsymbol{k}, \delta = \boldsymbol{k}'$, and summation over these repeated indices is implicitly understood.

Splitting the integral over τ into M imaginary time-slices and expanding the path integral measure into a product of individual integrals over specific quantum numbered and time-sliced Graßmann variables such that

$$\int \mathcal{D}[\xi^* \, \xi] \; \propto \; \lim_{M \to \infty} \int \prod_{\tau=1}^M \prod_\alpha \mathrm{d}\xi_{\alpha,\tau}^* \mathrm{d}\xi_{\alpha,\tau}, \tag{3.10}$$

the path-integral in Eq. (3.9) can be evaluated by the Gaussian Graß-
mann integral identity

$$\int \prod_i (\mathrm{d}\xi_i^* \mathrm{d}\xi_i) \, e^{-\xi_i^* S_{ij} \xi_j} = \det S, \qquad (3.11)$$

for which a derivation is found in Ref. [2]. This identity holds for any
Hermitian matrix S, even if it is not positive definite. The result is then
that the partition function in Eq. (3.9) becomes $\mathcal{Z} = \det S$. To calculate
this determinant one has to consider the matrix S as also a matrix with
time-slice indices. This is perhaps most easily accomplished using the
Matsubara formalism in which the τ dependence is substituted with
a dependence on Matsubara frequencies through a Fourier-like trans-
form.

3.1.3 Extended Nambu Spinor

From Eq. (3.8) we see that the Nambu spinor sesquilinear product fails
to accomodate terms in a Hamiltonian that mix creation and annihila-
tion operators of differing spins, e.g. a term $\propto \hat{c}_\uparrow^\dagger \hat{c}_\downarrow$. In general, a
quadratic Hamiltonian can contain any combination of spin-indices of
the form $\hat{c}_{s_1} \hat{c}_{s_2}$, $\hat{c}_{s_1}^\dagger \hat{c}_{s_2}$, $\hat{c}_{s_1} \hat{c}_{s_2}^\dagger$ and $\hat{c}_{s_1}^\dagger \hat{c}_{s_2}^\dagger$. This gives in total 16 dif-
ferent combinations and to accomodate them all we thus need a 4×4
matrix. Exchanging to Graßmann numbers we define the vector

$$\boldsymbol{\xi}_\gamma = \begin{pmatrix} \xi_{\gamma,\uparrow}^* \\ \xi_{\gamma,\uparrow} \\ \xi_{\gamma,\downarrow}^* \\ \xi_{\gamma,\downarrow} \end{pmatrix}, \qquad (3.12)$$

where all quantum numbers except spin is included in the index γ.
Writing the elements of this vector $(\boldsymbol{\xi}_\gamma)_i = \tilde{\xi}_{\gamma,i}$ regardless of whether
it is a conjugate or not, we can write all quadratic terms of a Hamilto-
nian on the bilinear form

$$\boldsymbol{\xi}_\gamma^{\mathsf{T}} S_{\gamma\delta} \boldsymbol{\xi}_\delta = \tilde{\xi}_{\gamma,i} S_{\gamma i; \delta j} \tilde{\xi}_{\delta,j}, \qquad (3.13)$$

where $S_{\gamma\delta}$ is a 4×4 anti-symmetric[2] matrix, and $S_{\gamma i; \delta j}$ denotes its
elements. Let there be n number of different quantum numbers, now

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2. To see why this matrix can always be said to be anti-symmetric lets first simplify
   the notation and write the bilinear product as $\tilde{\xi}_i S_{ij} \tilde{\xi}_j$. Then the matrix $S =$

including spin. Then there must be $2n$ different Graßmann genera-
tors $\tilde{\xi}_{\gamma,i}$. All of these are integrated over in the discrete version of the
partition function field integral

$$\mathcal{Z} = \int \mathcal{D}[\xi^* \, \xi] \; e^{- \int_0^\beta \mathrm{d}\tau \, \tilde{\xi}_{\gamma,i} S_{\gamma i; \delta j} \tilde{\xi}_{\delta,j}}. \tag{3.14}$$

Even though this superficially looks like the field integral in Eq. (3.9),
we now have a bilinear and not a sesquilinear form, and S is now a
$2n \times 2n$ matrix and not an $n \times n$ matrix. This means that we can not
use the integral in Eq. (3.11) to evaluate the integral but instead have
to rely on the more general Gaussian Graßmann integral

$$\int \prod_i (\mathrm{d}\tilde{\xi}_i) \; e^{-\frac{1}{2} \tilde{\xi}_i S_{ij} \tilde{\xi}_j} = \mathrm{Pf}(S), \tag{3.15}$$

which applies for any anti-symmetric matrix S. The right hand side
is called the Pfaffian $\mathrm{Pf}(S)$ of the matrix S and is defined for any anti-
symmetric matrix to be given by

$$\mathrm{Pf}[S] = \frac{1}{2^n n!} \sum_{P \in S_n} (-1)^P S_{P_1 P_2} \cdots S_{P_{n-1} P_n}, \tag{3.16}$$

where P is a permutation in the finite group S_n of all possible permu-
tations of n numbers. This matrix function is related to the determi-
nant by the relation $\mathrm{Pf}(S)^2 = \det(S)$.

Applying the integral identity in Eq. (3.15) to the partition function[3]
in Eq. (3.14) after applying the proper discretization of the imaginary

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$(S + S^\mathsf{T})/2 + (S - S^\mathsf{T})/2$, such that we can write it as a symmetric matrix
$\mathcal{S} = (S + S^\mathsf{T})/2$ and an anti-symmetric matrix $\mathcal{A} = (S - S^\mathsf{T})/2$. Considering
only the symmetric part of the bilinear form we get

$$\tilde{\xi}_i \mathcal{S}_{ij} \tilde{x} i_j = -\tilde{\xi}_j \mathcal{S}_{ij} \tilde{\xi}_i = -\tilde{\xi}_i \mathcal{S}_{ji} \tilde{\xi}_j = -\tilde{\xi}_i \mathcal{S}_{ij} \tilde{\xi}_j.$$

Hence $\tilde{\xi}_i \mathcal{S}_{ij} \tilde{\xi}_j = 0$ and all that remains is the antisymmetric bilinear form.

3. In relating the discrete version of Eq. (3.15) to (3.14) we have to make sure that
the spinor elements $\tilde{\xi}_i$ are defined in terms of ξ_i and ξ_i^* in such a way as to get a
correspondence to the sequence of Graßmann generators $\mathrm{d}\xi_i^* \mathrm{d}\xi_i$ in the measure
to avoid any sign errors. One solution is to set $\xi_i^* = \tilde{\xi}_{2i-1}$ and $\xi_i = \tilde{\xi}_{2i}$ as
we have done in Eq. (3.12). With this definition, then the measure $\int \prod_i \mathrm{d}\xi_i^* \mathrm{d}\xi_i$,
which results from the discretized version of the field-integral measure, becomes
equal to $\int \prod_{i=1}^{2n} \mathrm{d}\tilde{\xi}_i$ such that Eq. (3.15) can be directly applied.

time then yields the result

$$\mathcal{Z} = \int \mathcal{D}[\xi^* \, \xi] \, e^{-\int_0^\beta \mathrm{d}\tau \, \tilde{\xi}_{\gamma,i} S_{\gamma i; \delta j} \tilde{\xi}_{\delta,j}} = \sqrt{\det(S)}. \qquad (3.17)$$

We have chosen the positive result in $\mathrm{Pf}(S) = \pm\sqrt{\det(S)}$ since the partition function $\mathcal{Z}$ needs to be positive on physical grounds. The matrix S to be taken the derminant of on the right hand side of Eq. (3.17) is the full matrix one gets after discretizing the imaginary-time in slices which we usually have done through the Matsubara-frequency formalism.

Now that we know the partition function is given in terms of the determinant of the action-matrix S we can use this information to manipulate the definition of $\tilde{\xi}_{\gamma,i}$ so that we can still write the action as a sesquilinear form. In particular, switching the position of $\xi_{\gamma,s}^*$ and $\xi_{\gamma,s}$ for both spins in the transposed vector on the left of the bilinear form $\boldsymbol{\xi}_\gamma^\mathsf{T} S_{\gamma\delta} \boldsymbol{\xi}$, the transposed vector becomes the adjoint vector. This affects the matrix S by switching two pairs of rows. Denoting the matrix where the rows are switched S' then we have rewritten the bilinear form such that

$$\boldsymbol{\xi}_\gamma^\mathsf{T} S_{\gamma\delta} \boldsymbol{\xi}_\delta = \boldsymbol{\xi}_\gamma^\dagger S'_{\gamma\delta} \boldsymbol{\xi}_\delta. \qquad (3.18)$$

Now the integral over the exponent has not changed since all we have done is simply re-ordering its terms. However, since exchange of rows in a determinant at most produces a minus sign and we do this twice we get that $\det S = \det S'$ and we can write

$$\mathcal{Z} = \int \mathcal{D}[\xi^* \, \xi] \, e^{-\int_0^\beta \mathrm{d}\tau \, \boldsymbol{\xi}_\gamma^\dagger S'_{\gamma\delta} \boldsymbol{\xi}_\delta} = \sqrt{\det(S')}. \qquad (3.19)$$

where we need to remember that S' is the row switched matrix of an anti-symmetric matrix S.

3.2 Matsubara formalism

The Matsubara formalism[4] is a way of handling the imaginary time τ dependence of the coherent state eigenvalue fields $\xi_\alpha(\tau)$, where α denotes a collection of quantum numbers sufficient to specify a state, without having to go back to the time-sliced path-integral. It also lets

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4. Named after the Japanese physicst Matsubara, Takeo.

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us automatically satisfy the imaginary-time boundary conditions $\xi_\alpha(0) = \zeta \xi_\alpha(\beta)$, where $\zeta = +1$ for bosons and $\zeta = -1$ for fermions. Imagining that τ is a continuous variable as suggested in the path-integral notation, we define two countable infinite sets of new field-variables through the Fourier-transforms

$$\xi_{\alpha,n} = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \, e^{i\omega_n \tau} \xi_\alpha(\tau), \tag{3.20a}$$

$$\xi_{\alpha,n}^* = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \, e^{-i\omega_n \tau} \xi_\alpha^*(\tau). \tag{3.20b}$$

The frequencies ω_n are called Matsubara frequencies and are defined by $\omega_n = (2n+1)\pi/\beta$ with $n \in \mathbb{Z}$ for fermions. For bosons we use instead the notation ν_n where $\nu_n = 2n\pi/\beta$. The inverse relations are given by

$$\xi_\alpha(\tau) = \sum_{n \in \mathbb{Z}} e^{-i\omega_n \tau} \xi_{\alpha,n}, \tag{3.21a}$$

$$\xi_\alpha^*(\tau) = \sum_{n \in \mathbb{Z}} e^{i\omega_n \tau} \xi_{\alpha,n}^*. \tag{3.21b}$$

3.2.1 Matsubara sums

When the Matsubara formalism $\xi_{\alpha,n}$ is used for the field variables in the action of a partition-function field integral we will often need to evaluate infinite sums of Matsubara frequencies of the form

$$\sum_n h(if_n), \tag{3.22}$$

where f_n is either a fermionic or bosonic Matsubara frequency, to evaluate the field integral. A useful strategy in such evaluations is to transform the sum to a complex integral by using reverse residue integration. We consider the complex contour integral along a path $\mathcal{C}$ running counter-clockwise around the complex plane infinitesimally close to the imaginary axis as shown in Fig. 3.1. The integrand we consider is given by the product of the summand and the complex continuation of the Fermi-Dirac- or Bose-Einstein-distribution function

$$n_\zeta(z) = (e^{\beta z} - \zeta)^{-1}, \quad z \in \mathbb{C}, \tag{3.23}$$
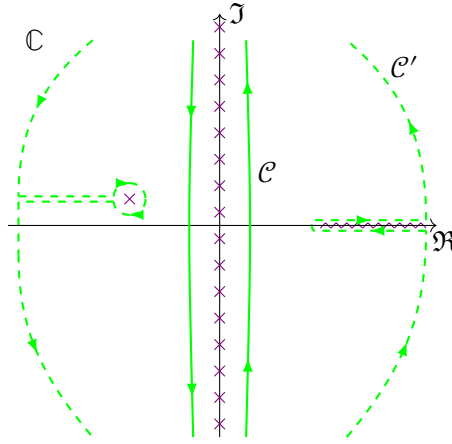
Figure 3.1: Integration contour for the Matsubara sum $\sum_n h(if_n)$. The contour is marked by a solid line and is imagined to continue to $\pm i\infty$. The crosses along the imaginary axis symbolizes the simple poles of the Fermi-Dirac distribution-function. A deformed integration contour is shown with dashed lines that is imagined to cross the real axis at $\pm\infty$. This contour then encloses a simple pole on the left and a branch cut on the right belonging to the summand.

depending on whether the Matsubara frequency in the sum is of fermionic ($\zeta = +1$) or bosonic ($\zeta = -1$) nature. This function has simple poles[5] at $z = if_n$ and thus integration around the contour results in a sum of residues of the integrand at these poles such that we get

$$\sum_n h(if_n) = \frac{\zeta\beta}{2\pi i} \oint_{\mathcal{C}} \mathrm{d}z \, h(z) n_\zeta(z), \qquad (3.24)$$

given that $h(z)$ does not contain any poles at these points. The contour can now be continuously deformed at will as long as it does not cross any singularities which can greatly facilitate the calculation of the integral. The default approach is to see if the integrand vanishes as $|z| \to \infty$, in which case it is usually useful to expand the contour as much as possible as illustrated by the deformed contour $\mathcal{C}'$ in Figure 3.1.

---

5. That the poles are simple, i.e. 1st order, is easily seen by expanding the exponential around if_n to leading order.

Using the method outlined above, we may calculate the sums

$$\sum_{n\in\mathbb{Z}}\frac{1}{if_n-x}=-\zeta\beta n_\zeta(x),\qquad\qquad(3.25\text{a})$$

$$\sum_{n\in\mathbb{Z}}\frac{1}{(i\omega_n-x)(i\omega_n-y)}=\frac{\beta}{x-y}\left(\frac{1}{1+e^{\beta x}}-\frac{1}{1+e^{\beta y}}\right),\quad(3.25\text{b})$$

$$\sum_{n\in\mathbb{Z}}\ln[\beta(i\omega_n+x)]=\ln(1+e^{-\beta x}).\qquad\qquad(3.25\text{c})$$

3.3 Hubbard-Stratonovich transformation

The Hubbard-Stratonovich transformation is a transformation in the fields of a theory where a new complex field is introduced in order to covert a term that is square and thus non-linear in an existing field variable, into a linear term in this variable that is coupled to the new field. This is particularly useful when the existing field is Fermionic and thus a Graßmann variable since it makes it possible to consider low energy exitations of the theory using e.g. a saddle-point approximation. It is however important to point out that the transformation itself is not in any way approximative, but is an exact transformation that maintains all information in the original theory.

In technical terms, the Hubbard-Stratonovich transformation can be viewed simply as the solution of a complex multivariate integral. Let A have a strictly positive Hermitian part and $\boldsymbol{J}$ be a vector of coefficients that could contain Graßmann variables or complex variables. Then

$$e^{\boldsymbol{J}^\dagger A\boldsymbol{J}}=\det A^{-1}\int_\mathbb{C}\prod_i\left[\frac{dz_i^*dz_i}{2\pi i}\right]e^{-(\boldsymbol{z}^\dagger A^{-1}\boldsymbol{z}+\boldsymbol{z}^\dagger\boldsymbol{J}+\boldsymbol{J}^\dagger\boldsymbol{z})},\qquad(3.26)$$

exchanges a quadratic term in $\boldsymbol{J}$ with a integration over the complex $\boldsymbol{z}$ variable. Since $\boldsymbol{J}$ usually represents some field in a field theory, the new $\boldsymbol{z}$ is called the auxhillary field or the conjugate field because of its linear coupling to $\boldsymbol{J}$. In the less general case that A is an Hermitian matrix, this formula is proved simply by completing the square, then diagonalizing A by a unitary tranformation and calculating the resulting integrals by the formula $\int_\mathbb{C}dz^*dz\,e^{-azz^*}=2\pi i/a$.

From Eq. (3.26) we see that what we have to do to perform the Hubbard-Stratonovich transformation is first to make a choice for what to interpret as part of the matrix A and what to interpret as part of $\boldsymbol{J}$.

We then have to check that this definition of A leads to its Hermitian part having only positive eigenvalues. Finally we need to know an analytical expression for its inverse. It is usually the first step that is the most difficult since this dictates the low energy excitation a subsequent saddle point approximation or a stationary phase approximation will produce. Typically we are interested in transforming a Fermionic interaction potential of the form

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \xi_\alpha^* \xi_\beta^* \xi_\delta \xi_\gamma, \tag{3.27}$$

where ξ_α are Graßmann variables, which can be sketched in the way of single-vertex diagram in Figure 3.2. The HS-transformation is clas-
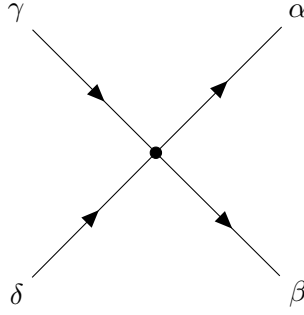
Figure 3.2: Generic two-body interaction.

sified into being done in a specific *channel* depending on which pair of Graßmann variables are considered to be part of $\boldsymbol{J}$ and consequently $\boldsymbol{J}^\dagger$. The direct channel[6] is given by the identification $J_i \sim \xi_\alpha^* \xi_\gamma$, the Cooper channel[7] is defined by the identification $J_i \sim \xi_\delta \xi_\gamma$ while the exchange channel is given by the identification $J_i \sim \xi_\alpha^* \xi_\delta$. Depending on exactly how $\boldsymbol{J}$ is chosen, the Gaussian integral in Eq. (3.26) might have to be modified. For example in the case of the direct- and exchange-channel, the exponential argument on the left side will have the form $\boldsymbol{J}^\mathsf{T} A \boldsymbol{J}$ which necessitates the Gaussian integral identity

$$e^{-\frac{1}{2} \boldsymbol{J}^\mathsf{T} A \boldsymbol{J}} = \sqrt{\det A^{-1}} \int_\mathbb{R} \prod_i \left[\frac{\mathrm{d}x_i}{\sqrt{2\pi}} \right] e^{-\frac{1}{2} \boldsymbol{x}^\mathsf{T} A^{-1} \boldsymbol{x} - i \boldsymbol{J}^\mathsf{T} \boldsymbol{x}}, \tag{3.28}$$

---

6. Also known as the density-density channel.
7. Also known as the particle-particle channel.

where the auxhillary field $\boldsymbol{x}$ now is a real conjugate field.

3.3.1 Transformation in symmetry channels

In the Cooper-channel of the Hubbard-Stratonovich transformation, the complex field $\boldsymbol{z}$ is conjugate to some combination of pairs of annihilation operators $\hat{c}_\delta \hat{c}_\gamma$ (or their corresponding Graßmann variables). The symmetry of the specific combination in turn then determines the symmetry of any low energy field theory obtained through a subsequent stationary phase approximation. By diagonalizing the interaction potential $\hat{V}$ into its particular irreducible representations as we did in Section 4.9 then a Hubbard-Stratonovich transformation in a specific symmetry channel is done by identifying $\boldsymbol{J}$ with irrep. basis functions.

Lets take the case of a BCS theory of superconductivity where the interaction can be written in terms of basis functions $d_{s_1 s_2}^{(b),m}(\boldsymbol{k})$ such that the diagonalized interaction takes the form

$$\hat{V} = \sum d_{s_1 s_2}^{(b),m}(\boldsymbol{k})^* v_{(b)} d_{s_1' s_2'}^{(b),m}(\boldsymbol{k}') c_{\frac{q}{2}+\boldsymbol{k}\, s_1}^\dagger c_{\frac{q}{2}-\boldsymbol{k}\, s_2}^\dagger c_{\frac{q}{2}-\boldsymbol{k}'\, s_2'} c_{\frac{q}{2}+\boldsymbol{k}'\, s_1'}, \tag{3.29}$$

where $\sum$ indicates the sum over the indices, $\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}, s_1, s_2, s_1', s_2', b$ and m. Here b specifies the irreducible representation while m enumerates the representation basis. Identifying

$$\hat{J}_{\boldsymbol{q}}^{(b_m)} = \sum_{\boldsymbol{k} s_1 s_2} d_{s_1 s_2}^{(b),m}(\boldsymbol{k}) \hat{c}_{\frac{q}{2}-\boldsymbol{k},s_1} \hat{c}_{\frac{q}{2}+\boldsymbol{k},s_2}, \tag{3.30}$$

the interaction potential is simply written

$$\hat{V} = \sum_{\boldsymbol{q},b,m} \hat{J}_{\boldsymbol{q}}^{(b_m)\,\dagger} v^{(b)} \hat{J}_{\boldsymbol{q}}^{(b_m)}. \tag{3.31}$$

In the path-integral representation of the partition function, the annihilation operators become Graßmann variables which we denote by writing J instead of $\hat{J}$ such that the contribution from the interaction potential results in the exponential

$$\mathcal{Z}_I = e^{-\int_0^\beta \mathrm{d}\tau \sum_{\boldsymbol{q},b,m} J_{\boldsymbol{q}}^{(b_m)\,\dagger} v^{(b)} J_{\boldsymbol{q}}^{(b_m)}}. \tag{3.32}$$

Now it is straight forward to use the Hubbard-Statonovich formula

$$e^{\int_0^\beta \mathrm{d}\tau \sum_{ij} J_i^* A_{ij} J_j} = \int \mathcal{D}[\eta_i^* \eta_i] e^{-\int_0^\beta \mathrm{d}\tau \left(\eta_i^* A_{ij}^{-1} \eta_j + J_i^* \eta_i + J_i \eta_i^* \right)}, \tag{3.33}$$

which is a path integral version of Eq. (3.26), to transform each pair of irreducible representation basis vectors to individual conjugate fields. In the notation of Eq. (3.33) implicit summation over repeated indices is used and each index i is a collection $i = (b, m, \boldsymbol{q})$ of indices. Comparing Eq. (3.33) and (3.32) we gather that

$$A_{ij} = A_{b,m,\boldsymbol{q}; \, b',m',\boldsymbol{q}'} = -\delta_{\boldsymbol{q}\boldsymbol{q}'}\delta_{mm'}\delta_{bb'}v^{(b)}, \qquad (3.34)$$

which is trivially Hermetic and positive definite provided $v^{(b)} < 0$. In this case we say that the irreducible representation b is an attractive channel. A is in this case also trivially invertible with $A_{ij}^{-1} = -\delta_{ij}/v^{(b)}$. Writing out all the indices we finally arrive at the Hubbard-Statonovich transformation of the interaction potential in individually attractive symmetry channels

$$\mathcal{Z}_I = \int \mathcal{D}[\eta_{\boldsymbol{q}}^{(b_m)*}\eta_{\boldsymbol{q}}^{(b_m)}]e^{\int_0^\beta d\tau \sum_{\boldsymbol{q} bm}\left[\frac{|\eta_{\boldsymbol{q}}^{(b_m)}|}{v^{(b)}} - \left(J_{\boldsymbol{q}}^{(b_m)*}\eta_{\boldsymbol{q}}^{(b_m)} + J_{\boldsymbol{q}}^{(b_m)}\eta_{\boldsymbol{q}}^{(b_m)}\right)\right]},$$

$$(3.35)$$

where

$$J_{\boldsymbol{q}}^{(b_m)} = \sum_{\boldsymbol{k}\, s_1 s_2} d_{s_1 s_2}^{(b),m}(\boldsymbol{k})\xi_{\frac{\boldsymbol{q}}{2}-\boldsymbol{k},s_1}\xi_{\frac{\boldsymbol{q}}{2}+\boldsymbol{k},s_2} \qquad (3.36)$$

in terms of Graßmann variables ξ. We note that this derivation does not assume either odd or even basis functions for the irreducible representations and works just as well for either.

3.4 Field theory approximations

3.4.1 Stationary phase and the one loop expansion

Let Z be the partition function

$$Z(l) = \int \mathcal{D}[\eta_\alpha^*\,\eta_\alpha]\, e^{-lS(\eta_\alpha^*,\eta_\alpha)}, \qquad (3.37)$$

given in terms of bosonic fields $\eta_\alpha^*, \eta_\alpha$ and where l is some large parameter $l \gg 1$. In what is called the stationary phase approximation[8]

---

8. The name is misleading in the case of the many-particle partition function since we do not have a strict phase in the exponent but in general a complex function because $\eta_\alpha \in \mathbb{C}$. Technically it is the method of steepest descent in the case of an exponent with stationary points that is used in this case.

of a bosonic field integral we create an expansion of the free energy around the field configuration $\{\eta^c_\alpha\}$ where the action S is stationary and a minimum. This configuration is the main contribution to the integral in Eq. (3.37) since it provides the maximum of the exponent, and determines the leading order asymptotic behavior as $l \to \infty$. It also corresponds in a sense to a classical solution and gives in the case of the feynman path integral for the evolution operator of a single particle in an external potential, the classical Euler-Lagrange equations. The configuration is found in the path-integral notation by varying the fields in the action such that

$$\frac{\delta S}{\delta \eta_\alpha} = 0 \quad \wedge \quad \frac{\delta S}{\delta \eta^*_\alpha} = 0. \tag{3.38}$$

As an example, the Hubbard-model can be expressed by a bosonic field integral through a Hubbard-Statonovich transformation. The stationary field configuration $\{\eta^c_q(\tau)\}$ is in this case given by a imaginary-time- and spatialy-independent field-configuration η^c. Assuming such a solution, the action reduces to

$$S(\eta^{c\,*}, \eta^c) = \frac{\beta N}{U} |\eta^c|^2 - \sum_q \ln \left[\left(1 + e^{\beta E_q} \right) \left(1 + e^{-\beta E_q} \right) \right], \tag{3.39}$$

where $E_q = \sqrt{(\epsilon(q) - \mu)^2 + |\eta^c|^2}$, N is the number of hopping sites, $\epsilon(q)$ is the Fourier transformed kinetic hopping energy, μ is the chemical potential, and U is the repulsive Hubbard interaction strength. The stationary action condition in Eq. (3.38) then yields the equation

$$|\eta^c| \left(\frac{1}{U} - \frac{1}{N} \sum_q \frac{1}{2E_q} \tanh \frac{\beta E_q}{2} \right) = 0, \tag{3.40}$$

which has two solution: one given by $\eta^c = 0$ and one given by setting the terms in parenthesis equal to 0. The last non-trivial solution is a form of the BCS solution and represents the order-parameter in an s-wave superconductor. Because of the parameter β, this solution will be temperature dependent and dissapears at some critical temperature at which the two solutions for η_c converge.

The stationary phase expansion is then the expansion resulting from expanding the action around the stationary solution. Setting $\tilde{\eta}_\alpha =$

$\sqrt{l}(\eta_\alpha - \eta_\alpha^c)$ we get in general the expansion

$$
\begin{aligned}
S(\tilde{\eta}_\alpha, \tilde{\eta}_\alpha^*) = S_c &+ \frac{1}{l}\left[\frac{1}{2!} \frac{\delta^2 S}{\delta\eta_\alpha \delta\eta_\beta}\bigg|_{\eta_c} \tilde{\eta}_\alpha \tilde{\eta}_\beta \right.\\
&+ \left. \frac{1}{2!} \frac{\delta^2 S}{\delta\eta_\alpha^* \delta\eta_\beta^*}\bigg|_{\eta_c} \tilde{\eta}_\alpha^* \tilde{\eta}_\beta^* + \frac{\delta^2 S}{\delta\eta_\alpha \delta\eta_\beta^*}\bigg|_{\eta_c} \tilde{\eta}_\alpha \tilde{\eta}_\beta^* \right] + \mathcal{O}\left(\frac{1}{l\sqrt{l}}\right)\\
&= \sum_{n_1+n_2\geq 2} \frac{1}{n_1! n_2!} \frac{\delta^{n_1+n_2} S}{\delta\tilde{\eta}_\alpha^{n_1} \delta\tilde{\eta}_\beta^{* \, n_2}} \tilde{\eta}_\alpha^{n_1} \tilde{\eta}_\beta^{* \, n_2}\bigg|_{\eta_c} \frac{1}{l^{(n_1+n_2)/2}}.
\end{aligned}
$$
(3.41)

We have used implicit summation over repeated indices and on the last line we have assumed that new indices should be introduced and summed for each n_1 and n_2. This is simply the multivariate Taylor expansion around η_c where we have treated η and η^* as independent variables.

A simpler expansion can be found when the bosonic fields correspond to order parameters in a system close to a phase transition. In this case we can assume the fields η_α to be small in general such that S simply can be expanded about 0. If the system is fermionic, then the bosonic field integral of the order-parameters will have resulted from a Hubbard-Stratonovich transformation, in which case we will have a contribution to the integral of the form

$$
\sqrt{\det G^{-1}(\eta_\alpha, \eta_\alpha^*)} = e^{\frac{1}{2}\operatorname{Tr}\ln G^{-1}},
$$
(3.42)

where G^{-1} is the result of the integration of a quadratic fermionic action, and will in general depend on the auxhillary bosonic fields η_α and η_α^* in a linear way. Then the matrix G^{-1} can be decomposed in a matrix G_0^{-1} that results purely from fermionic integration, and a matrix ϕ that is dependent on the auxhillary fields η_α and importantly vanishes as $\eta_\alpha \to 0$, such that $G^{-1} = G_0^{-1} + \phi$. When the system is close the the phase transition such that the auxhillary fields are small, then this allows for the expansion of the logarithm in Eq. (3.42) such that

$$
\begin{aligned}
\frac{1}{2}\operatorname{Tr}\ln(G_0^{-1} + \phi) &= \frac{1}{2}\left(\operatorname{Tr}\ln G_0^{-1} + \operatorname{Tr}\ln(1 + G_0\phi) \right)\\
&= \frac{1}{2}\left(\operatorname{Tr}\ln G_0^{-1} - \sum_{n=1}^{\infty} \frac{\operatorname{Tr}(-G_0\phi)^n}{n} \right).
\end{aligned}
$$
(3.43)

This is known as the one-loop expansion since in terms of perturbation theory, G_0 is the fermionic propagator such that the sum in the last line of Eq. (3.43) corresponds to a series of propagators and interactions that are connected in a closed loop by the trace.

3.4.2 Gradient expansion

The gradient expansion rests on the assumption that the fields are sufficiently smooth such that progressively higher order derivatives with respect to the field parameters, are progressively smaller, i.e. we assume

$$l_\alpha^n |\partial_\alpha^n \eta_\alpha| \gg l_\alpha^{n+1} |\partial_\alpha^{n+1} \eta_\alpha|, \tag{3.44}$$

where l_α is some appropriate length scale such as to make $l_\alpha \partial_\alpha$ dimensionless. In practice this usually means that given a momentum-dependent action density, $S(\eta_{\boldsymbol{q},\alpha}^*, \eta_{\boldsymbol{q},\alpha}; \boldsymbol{q})$, we assume q_i small compared to the lattice spacing[9] a_i. Then we expand the explicit $\boldsymbol{q}$ dependence in the action density in the small parameters $a_i q_i$ as a McLaurien series. In the following notation, we will assume the length parameter a^i is present in the notation q^i where appropriate. The momentum dependence of the fields themselves should not be expanded as our goal is terms of the form $(q^i)^n (\tilde{\eta}_{\boldsymbol{q},\alpha})^m$. If we then let partial momentum-derivatives only act on the explicit momentum-dependence in S, and neglecting the field dependence in the notation for S, the expanded action can be written as the series

$$S(\boldsymbol{q}) = S(0) + \frac{\partial S}{\partial q^i}(0)\, q^i + \frac{1}{2!} \frac{\partial^2 S}{\partial q^i \partial q^j}(0)\, q^i q^j + \mathcal{O}(q^3). \tag{3.45}$$

Usually, the linear term cancels by symmetry of the underlying lattice. In general it is smart to here check for terms that cancel by considering any internal momentum sums that may be included in the coefficients.

Terms with products between fields $\eta_{\boldsymbol{q},\alpha}$ and q^i lead to gradients of the spatially dependent fields $\eta_{\boldsymbol{R},\alpha}$, which is why the expansion in Eq. (3.45) can be called a gradient expansion. The spatially dependent fields are defined as the coefficients in the inverse Fourier transform

$$\eta_{\boldsymbol{q},\alpha} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}} \eta_\alpha(\boldsymbol{R}), \tag{3.46}$$

---

9. This could be the spacing between hopping sites, i.e. stationary ions in an electron model.

where N is the number of terms in the sums $\sum_{\boldsymbol{q}}$ and $\sum_{\boldsymbol{R}}$. One way of now obtaining gradients of the spatial fields is to realize that since q^i is small we can set

$$q^i \approx \sin(q^i) = \frac{1}{2i}\left(e^{iq^i} - e^{-iq^i} \right). \tag{3.47}$$

With this identification, all the momentum dependence in $S(\boldsymbol{q})$ exists as phases such that the sum $\sum_{\boldsymbol{q}} S(\boldsymbol{q})$ results in a series of Kronicker-delta functions which we evaluate by the $\sum_{\boldsymbol{R}}$ sums coming from the inverse Fourier transforms in Eq. (3.46). Grouping terms of displaced spatial fields, we can identify derivaties, such that

$$\eta_\alpha(\boldsymbol{R} + a\hat{e}_i) - \eta_\alpha(\boldsymbol{R}) \approx a\frac{\partial}{\partial R^i}\eta_\alpha(\boldsymbol{R}). \tag{3.48}$$

These identifications are justified by going to the continuum limit where $a \to 0$.

As an example, consider the sum

$$S = \sum_{\boldsymbol{q}} K_{\alpha\beta ij}q^i q^j \eta^*_{\boldsymbol{q},\alpha}\eta_{\boldsymbol{q},\beta}, \tag{3.49}$$

where there is an implicit summation over repeated indices i, j, α and β. Fourier transforming the fields according to Eq. (3.46) and writing q^i as $\sin q^i$, we can group terms such that

$$S = \frac{1}{N}\sum_{\boldsymbol{R}_1 \boldsymbol{R}_2} K_{\alpha\beta ij}\eta_\alpha(\boldsymbol{R}_1)^*\eta_\beta(\boldsymbol{R}_2)\frac{1}{4}\sum_{\boldsymbol{q}}\left[e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_2 - \boldsymbol{R}_1 + a\hat{e}_i - a\hat{e}_j)} \right.$$
$$+ e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_2 - \boldsymbol{R}_1 + a\hat{e}_j - a\hat{e}_i)} - e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_2 - \boldsymbol{R}_1 + a\hat{e}_i + a\hat{e}_j)} - e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_2 - \boldsymbol{R}_1 - a\hat{e}_i - a\hat{e}_j)} \Big]$$
$$= \sum_{\boldsymbol{R}} K_{\alpha\beta ij}a^2\frac{\partial}{\partial R_i}\eta_\alpha(\boldsymbol{R})^*\frac{\partial}{\partial R_j}\eta_\beta(\boldsymbol{R}). \tag{3.50}$$

A more conventional way of converting to gradients, is to use integration by parts. Then the product rule of partial derivatives is used to obtain

$$q^j\eta_\alpha(\boldsymbol{R})e^{i\boldsymbol{q}\cdot\boldsymbol{R}} = i\frac{\partial\eta_\alpha}{\partial R^i}e^{i\boldsymbol{q}\cdot\boldsymbol{R}} - i\frac{\partial}{\partial R^i}\left[\eta_\alpha(\boldsymbol{R})e^{i\boldsymbol{q}\cdot\boldsymbol{R}} \right]. \tag{3.51}$$

Summing on both sides and arguing that the bounary term vanishes because $\eta_\alpha(\boldsymbol{R}) \to 0$ as $R^i \to \infty$, then

$$\sum_{\boldsymbol{R}} q^j\eta_\alpha(\boldsymbol{R})e^{i\boldsymbol{q}\cdot\boldsymbol{R}} = i\sum_{\boldsymbol{R}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}}\nabla_i\eta_\alpha(\boldsymbol{R}). \tag{3.52}$$

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

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

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 $\sigma^0 = \mathbb{1}_{2\times2}$, 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

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

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

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

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

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

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

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

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

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 $\{\bm{b}_i\}_{i=1}^d$. The application of a group element to a basis vector is then defined as

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

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:

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

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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 $|\boldsymbol{k}\rangle$ 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 $|\boldsymbol{k}, s\rangle = |\boldsymbol{k}\rangle|s\rangle$. Given $\boldsymbol{k} \in \mathbb{R}^d$ and $s \in \{\uparrow, \downarrow\}$, these basis vectors transform according to the product representation of the representations on each vector space, given by

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

under a group element g. Here $g\boldsymbol{k}'$ means application of g to the vector $\boldsymbol{k}'$ 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

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

where $\hat{\boldsymbol{u}}$ 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: $\{|\boldsymbol{k}, s_1\rangle|-\boldsymbol{k}, s_2\rangle\}$. The product representation on this vector space then transforms the basis vectors according to

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

$$(4.26)$$

where

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

Since group representations on $\boldsymbol{k}$ is a linear transformation then $\delta_{-\boldsymbol{k}, g:-\boldsymbol{k}'} = \delta_{\boldsymbol{k}, g:\boldsymbol{k}'}$, 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

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

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

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

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

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

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

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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.

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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 $y = -x$

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

	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

4.7.1 Conjugation classes

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 $e = \{e\}$, $2C_4 = \{C_4, C_4^{-1}\}$, $C_4^2 = \{C_4^2\}$, $2\sigma_d = \{\sigma_{d_1}, \sigma_{d_2}\}$ 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

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

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 with-

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

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

out knowing the details of the irreducible representations but in stead using character relations from basic group theory.[2]

4.7.2 Irreducible representations

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 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 ma-

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2. Many of these relations are derived from the great orthogonality theorem which can be found e.g. in [3].

trices

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

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

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

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

Taking the trace of these matrices, we see that this representations characters are the same as the ones for the irrep. Γ_5 in the character table (Table 4.2). This implies that $\sum_g |\chi^{\Gamma_5 u}(g)|^2 = |C_{4_v}|$ which implies in turn that the representation given by the matrices in Eq. (4.44) is irreducible. Thus this is indeed the Γ_5 irreducible representation as advertised, and we have completed the description of the representation matrices of all the irreducible representations of C_{4v}.

4.7.3 Representation on odd BCS functions d_k

When discussing the representation of general group elements on states in the BCS Hilbert space in Section 4.4.3 we learned from Eq. (4.35) that the coefficient $d_k \in \mathbb{R}^3$ of odd states transforms by a proper rotation $R(\hat{u}, \phi)$. A proper rotation of a group element g is the rotation obtained when writing g as a rotation followed by an inversion P or identity. We thus obtain the representation matrices of the 3D-representation of group elements $g \in C_{4v}$ directly from the 3D rotation matrix $R(\hat{u}, \phi)$ by envisioning the combination of a rotation and $C_4^2 = P$ or e that leads to g. Because of this, we denote the representation matrices of this representation $R(g)$. As an example $\sigma_x = C_4^2 R(\hat{x}, \pi)$, such that the representation $R(\sigma_x) = R(\hat{x}, \pi)$. Written out in its full matrix form this yields the representation matri-

ces

$$R(C_4) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad R(C_4^{-1}) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \text{(4.45a)}$$

$$R(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad R(C_4^2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \text{(4.45b)}$$

$$R(\sigma_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad R(\sigma_y) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad \text{(4.45c)}$$

$$R(\sigma_{d_1}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad R(\sigma_{d_2}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

$$\text{(4.45d)}$$

4.8 Square Lattice Harmonics

Since $\psi(\mathbf{k})$ and $\mathbf{d_k}$ are invariant with respect to translation by any re-siprocal lattice vector $\mathbf{Q}$: $\psi(\mathbf{k} + \mathbf{Q}) = \psi(\mathbf{k})$, they can be expanded in a discrete Fourier transform over the real lattice, such that

$$\psi(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \psi_{\mathbf{R}} \cos \mathbf{R} \cdot \mathbf{k}, \qquad \text{(4.46)}$$

and

$$\mathbf{d_k} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \mathbf{d_R} \sin \mathbf{R} \cdot \mathbf{k}, \qquad \text{(4.47)}$$

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 $\psi(\mathbf{k})$ and $\mathbf{d_k}$ for even and odd bases respectively. 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

We remember from Eq. (4.29) that the function $\psi(\boldsymbol{k})$ transforms as g : $\psi(\boldsymbol{k}) = \psi(g^{-1} : \boldsymbol{k})$ under a group transformation g. Operating on the Fourier expansion of $\psi(\boldsymbol{k})$ in Eq. (4.46) with the projection operator defined in Eq. (4.38) by an arbitrary irrep. Γ yields

$$
\begin{aligned}
P_{l,l}^{(\Gamma)}\psi(\boldsymbol{k}) = \frac{d_\Gamma}{8\sqrt{N}} \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \Big[& (D_{ll}^{(\Gamma)}(e) + D_{ll}^{(\Gamma)}(C_4^2)) \cos(\boldsymbol{R} \cdot \boldsymbol{k}) \\
& + (D_{ll}^{(\Gamma)}(C_4) + D_{ll}^{(\Gamma)}(C_4^{-1})) \cos(R_x k_y - R_y k_x) \\
& + (D_{ll}^{(\Gamma)}(\sigma_x) + D_{ll}^{(\Gamma)}(\sigma_y)) \cos(R_x k_x - R_y k_y) \\
& + (D_{ll}^{(\Gamma)}(\sigma_{d_1}) + D_{ll}^{(\Gamma)}(\sigma_{d_2})) \cos(R_x k_y + R_y k_x).
\end{aligned}
$$
(4.48)

Since $\boldsymbol{k} \in \mathbb{R}^2$ we have in this calculation used the natural $2D$ representation given by the matrices in Eq. (4.44) of the group elements in C_{4v} to calculate the expressions $g^{-1} : \boldsymbol{k}$ inside the cosine functions. Inserting the matrix element of the different irreducible representations of C_{4v} which we discussed in Section 4.7 we get the projected functions

$$
\begin{aligned}
P_{1,1}^{(\Gamma_1)}\psi(\boldsymbol{k}) &\propto \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \big[\cos R_x k_x \cos R_y k_y + \cos R_x k_y \cos R_y k_x \big], \\
P_{1,1}^{(\Gamma_2)}\psi(\boldsymbol{k}) &\propto \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \big[\sin R_x k_y \sin R_y k_x - \sin R_x k_x \sin R_y k_y \big], \\
P_{1,1}^{(\Gamma_3)}\psi(\boldsymbol{k}) &\propto \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \big[\cos R_x k_x \cos R_y k_y - \cos R_x k_y \cos R_y k_x \big], \\
P_{1,1}^{(\Gamma_4)}\psi(\boldsymbol{k}) &\propto \sum_{\boldsymbol{R}} \psi_{\boldsymbol{R}} \big[\sin R_x k_x \sin R_y k_y + \sin R_x k_y \sin R_y k_x \big], \\
P_{1,1}^{(\Gamma_5)}\psi(\boldsymbol{k}) &\propto 0, \\
P_{2,2}^{(\Gamma_5)}\psi(\boldsymbol{k}) &\propto 0.
\end{aligned}
$$
(4.49)

Since the projection operators $P_{ll}^{(\Gamma)}$ projects onto the subspace of vectors belonging to the irreducible representation Γ, if we let the different

basis functions of the irreps. Γ be denoted $\psi^{(\Gamma),q,m}(\boldsymbol{k})$, then we expect the projection to produce the result

$$P_{l,l}^{(\Gamma)}\psi(\boldsymbol{k}) = \sum_q c_{q,l}\psi^{(\Gamma),q,l}(\boldsymbol{k}). \qquad (4.50)$$

Here q again enumerates the version of the basis of Γ possible in the space of different $\psi(\boldsymbol{k})$, and $c_{q,l}$ are the coefficients of $\psi(\boldsymbol{k})$ in the basis of the irrep. basis functions. Comparing Eqs. (4.50) and (4.49), we see that different sets of basis vectors can be obtained for the irreducible representations by including different order terms in the $\boldsymbol{R}$-sum, i.e. different lattice neighbour sites. It is also worth noting that the irreducible representation Γ_5 does not exist in the space of possible $\psi(\boldsymbol{k})$, since it is an odd representation.

Including on-site, nearest neighbor and next-nearest neighbor sites in the $\boldsymbol{R}$ sum of the projected arbitrary function $\psi(\boldsymbol{k})$ on the Γ_1 subspace in Eq. (4.50) we see that any such function can be constructed from the three basis functions

$$\psi^{(\Gamma_1),1}(\boldsymbol{k}) = \frac{1}{2\pi}, \qquad (4.51a)$$

$$\psi^{(\Gamma_1),2}(\boldsymbol{k}) = \frac{1}{2\pi}(\cos k_x + \cos k_y), \qquad (4.51b)$$

$$\psi^{(\Gamma_1),3}(\boldsymbol{k}) = \frac{1}{\pi}\cos k_x \cos k_y. \qquad (4.51c)$$

Each of these functions give a complete basis function set of the Γ_1 irreducible representation which can be checked by calculating how they transform under group elements $g \in C_{4v}$. In this case, since this is the trivial Γ_1 representation, the functions are symmetric under all group elements g which produces the character 1 for all conjugation classes (compare with first row in Table 4.2).

These basis functions are automatically mutually orthogonal since they belong to different irreducible representation version subspaces and their normalization coefficients have been chosen such that they are normal on the 1$^{\text{st}}$ Brillouin zone, i.e.

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}k_x \mathrm{d}k_y \, \psi^{(\Gamma_1),q}(\boldsymbol{k})^*\psi^{(\Gamma_1),q'}(\boldsymbol{k}) = \delta_{qq'}. \qquad (4.52)$$

Inserting up to next-nearest neighbor sites for $\boldsymbol{R}$ in the projected functions under the remaining irreducible representations we find the

orthonormal basis functions

$$\psi^{(\Gamma_3)}(\boldsymbol{k}) = \frac{1}{2\pi}(\cos k_x - \cos k_y), \qquad (4.53\text{a})$$

$$\psi^{(\Gamma_4)}(\boldsymbol{k}) = \frac{1}{\pi}\sin k_x \sin k_y, \qquad (4.53\text{b})$$

of the representations Γ_3 and Γ_4 respectively. The Γ_3 basis is found by expansion of $\boldsymbol{R}$ to nearest neighbor, while the one for Γ_4 is found at next-nearest neighbor. To get a basis vector for the representation Γ_2 we would need to expand beyond the next-nearest neighbor site.

These basis functions are also known as square lattice harmonics. The set of square lattice harmonic functions includes the set of functions found when expanding $\boldsymbol{R}$ to arbitrary sites. As we have seen, they can be grouped and found through consideration of the irreducible representations of the symmetry group of the square lattice. We have so far only considered even-in-$\boldsymbol{k}$ basis functions. In the next section we will complete our discussion of square lattice harmonics with the inclusion of odd functions.

4.8.2 Odd basis functions

Any state made out of odd basis functions is fully determined by the coefficients $\boldsymbol{d_k}$. These coefficients transform as $g : \boldsymbol{d_k} = R(g)\boldsymbol{d}_{g^{-1}:\boldsymbol{k}}$ under group elements $g \in C_{4v}$, see Eq. (4.35), where $R(g)$ are the representation matrices in Eq. (4.45). Acting on the Fourier expansion of the arbitrary function $\boldsymbol{d_k}$ in Eq. (4.47) with the projection operators Eq. (4.38) down on the subspace of the irreducible representation Γ_5 of the symmetry group C_{4v} yields the results

$$P_{1,1}^{(\Gamma_5)}\boldsymbol{d_k} = \frac{\hat{\boldsymbol{z}}}{\sqrt{N}}\sum_{\boldsymbol{R}} d_{\boldsymbol{R},z}\cos R_x k_x \sin R_y k_y, \qquad (4.54\text{a})$$

$$P_{2,2}^{(\Gamma_5)}\boldsymbol{d_k} = \frac{\hat{\boldsymbol{z}}}{\sqrt{N}}\sum_{\boldsymbol{R}} d_{\boldsymbol{R},z}\sin R_x k_y \cos R_y k_y, \qquad (4.54\text{b})$$

for the two basis functions of Γ_5. As in the spin-singlet case we get different versions of the Γ_5 basis vectors depending on the order of our expansion in $\boldsymbol{R}$. Expanding to nearest neighbor sites and normalizing

such that the states are orthonormal produces the basis functions

$$d_{\boldsymbol{k}}^{(\Gamma_5),1} = -\frac{\hat{\boldsymbol{z}}}{2\pi} \sin k_y, \qquad (4.55a)$$

$$d_{\boldsymbol{k}}^{(\Gamma_5),2} = \frac{\hat{\boldsymbol{z}}}{2\pi} \sin k_x, \qquad (4.55b)$$

of the two-dimensional irreducible representation Γ_5.

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

$$\hat{V}|\alpha_1\rangle ... |\alpha_N\rangle = \sum_{1 \le i < j \le N} \hat{V}_{ij}|\alpha_1\rangle ... |\alpha_N\rangle, \qquad (4.56)$$

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

$$\langle\alpha|\langle\alpha'|\hat{V}|\beta\rangle|\beta'\rangle. \qquad (4.57)$$

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

$$V_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \boldsymbol{k}_4; s_1 s_2 s_3 s_4} = \langle \boldsymbol{k}_1 s_1 | \langle \boldsymbol{k}_2 s_2 | \hat{V} | \boldsymbol{k}_4 s_4 \rangle | \boldsymbol{k}_3 s_3 \rangle. \qquad (4.58)$$

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

$$V_{\boldsymbol{k}\boldsymbol{k}'; s_1 s_2 s_3 s_4} = \langle \boldsymbol{k} s_1 | \langle -\boldsymbol{k} s_2 | \hat{V} | \boldsymbol{k}' s_4 \rangle | -\boldsymbol{k}' s_3 \rangle. \qquad (4.59)$$

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

$$\hat{V} = \sum_{\Gamma q_\Gamma} V_{\Gamma, q_\Gamma} \sum_{m=1}^{d_\Gamma} |\Gamma, q_\Gamma, m\rangle\langle\Gamma, q_\Gamma, m|. \qquad (4.60)$$

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. (4.59) lets us write them in terms of irreducible representation basis vectors in the momentum spin function representation:

$$V_{\boldsymbol{k}\boldsymbol{k}'; s_1 s_2 s_3 s_4} = \sum_{\Gamma} V_{\Gamma, q_\Gamma} \sum_{m=1}^{d_\Gamma} \Psi_{s_1 s_2}^{\Gamma, q_\Gamma}(\boldsymbol{k})\Psi_{s_3 s_4}^{\Gamma, q_\Gamma}(-\boldsymbol{k}')^\dagger, \qquad (4.61)$$

where

$$\Psi_{s_1 s_2}^{\Gamma, q_\Gamma}(\boldsymbol{k}) = \langle \boldsymbol{k}, s_1|\langle -\boldsymbol{k}, s_2 \mid \Gamma, q_\Gamma, m\rangle. \qquad (4.62)$$

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

$$\Psi_{s_1 s_2}^{a,q_a,m}(\boldsymbol{k}) = \psi_{\boldsymbol{k}}^{a,q_a,m} i\sigma_{s_1 s_2}^{y}. \tag{4.63}$$

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

$$\Psi_{s_1 s_2}^{b,q_b,m}(\boldsymbol{k}) = \boldsymbol{d}_{\boldsymbol{k}}^{b,q_b,m} \cdot (\boldsymbol{\sigma} i\sigma^{y})_{s_1 s_2}. \tag{4.64}$$

Separating the sum over irreducible representations Γ into sums over even (a) and odd (b) representations in the potential operator matrix elements in Eq. (4.61), we arrive at the fully expanded expression

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

$$+ \sum_{b q_b} V_{b,q_b} \sum_{m=1}^{d_b} \big(\boldsymbol{d}_{\boldsymbol{k}}^{b,q_b,m} \cdot \boldsymbol{\sigma} i\sigma^{y}\big)_{s_1 s_2} \Big[\big(\boldsymbol{d}_{-\boldsymbol{k}'}^{b,q_b,m} \cdot \boldsymbol{\sigma} i\sigma^{y}\big)_{s_3 s_4}\Big]^{\dagger}. \tag{4.65}$$

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 $\sigma_{s_1 s_2}^{\dagger} = \sigma_{s_2 s_1}^{*}$.

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. In such systems these techniques wil be used to calculate thermal averages using random numbers. Let Z denote the partition function and $\mathcal{H}$ the Hamiltonian of the system. Then the thermal average of an observable $\mathcal{O}$ is defined as

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{\psi} \mathcal{O}(\psi) e^{-\beta \mathcal{H}(\psi)}, \tag{6.1}$$

where ψ denotes states of the system.

6.1 Markov-Chain Monte-Carlo method

6.2 Metropolis-Hastings method

6.3 Importance sampling of observables

6.4 Thermalization procedures

6.5 Parallell tempering

6.6 Reweighting

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 [4–6].

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.

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

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

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

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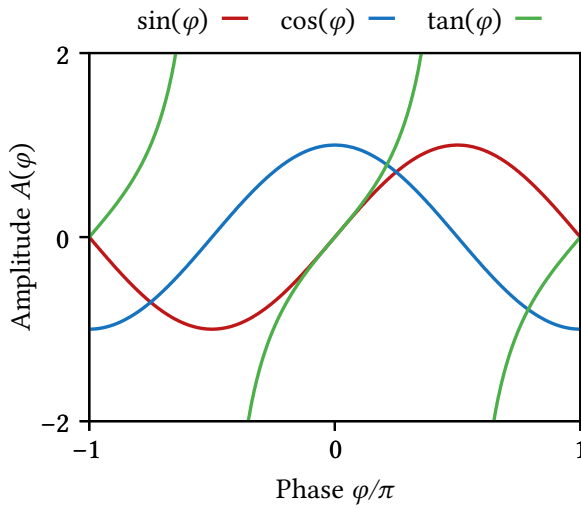
Figure 8.1: This is an example figure made by GNUPLOT. I have also included an intentionally long caption to show the margins.

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

8.2 Lorem ipsum

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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	$\sqrt{-1}$

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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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