

Chapter 2

Weak Coupling Theory

2.1 Introduction

It is widely believed that the main difference between conventional and unconventional superconductors is that correlations arising from the repulsion between electrons plays a key role in the latter case and is thought to, at least partially, replace phonons as the microscopic source for electron pairing. It might seem counterintuitive at first that a repulsive interaction between electrons could lead to the formation of Cooper pairs. The idea is that the electron-electron interaction can become effectively attractive due to various screening mechanisms, although the identification of this mechanism is still a matter of debate [1]. Since it was shown by BCS that even a vanishingly small attractive interaction between electrons close to the Fermi level is enough to trigger superconductivity [2], the crux of the problem is to find a microscopic mechanism which screens the bare repulsive interaction enough so that it becomes attractive in some channel. While the details differ, this electronic mechanism for superconductivity is always related to the screening of the bare interaction due to fluctuations of the Fermi liquid [3].

The first proposal for such an electronic mechanism for superconductivity was given by Kohn and Luttinger [4]. They computed the screened interaction perturbatively in the weak interaction limit for a homogeneous electron gas with short-range interactions. Since this problem has rotational invariance, the effective interaction can be decomposed in angular momentum channels. They then showed that, thanks to a singularity at momentum $2k_F$ (k_F is the Fermi momentum) in the second derivative of the Lindhard (or bare) particle-hole susceptibility (defined below) of the 3D free electron gas, regardless of the form of the interaction, there will always be at least one angular momentum channel in which the interaction is attractive. Cooper pairs will then form in that channel. The BCS instability is therefore inevitable for a uniform 3D electron gas with short-range interactions. Note that even though this is strictly true, the critical temperature T_c can be extremely small since it scales like

$$\frac{T_c}{E_F} \sim e^{-(2l)^4} \quad (2.1)$$

where E_F is the Fermi energy and l is the total angular momentum quantum number ($l = 0$ for s-wave, $l = 1$ for p-wave, ...).

Since the screened interaction is computed perturbatively in the Kohn-Luttinger method, it is exact only in the vanishing interaction limit. It is possible to study superconductivity in this limit thanks to the fact that, unlike for other instabilities like charge and spin density waves, there is no threshold value of the interaction below which the Fermi liquid is stable: Even a vanishingly small interaction will drive superconductivity [4, 5]. Despite the fact that interactions are actually strong in realistic systems, this method was successfully applied to several unconventional superconductors, like cuprates, pnictides and organic superconductors (for a review, see Ref. [3]).

In essence, the calculation developed in this Chapter is a generalization of Kohn and Luttinger's work to the generic case of a multi-band, spin-orbit coupled superconductor on a lattice. The screened interaction will be calculated perturbatively in the weak interaction limit and will be expressed in terms of the bare particle-hole susceptibility, generalized to the multi-orbital case. Unlike in the homogeneous electron gas case, this susceptibility is not known analytically and has to be computed numerically. Furthermore, since lattice systems do not have rotational invariance, an important difference is that the different possible order parameters are classified according to the point group of the lattice instead of angular momentum.

Superconductivity can also be studied at finite interaction. Spin fluctuations can be greatly enhanced by interactions close to a magnetic transition. Within the random phase approximation [6], the bare particle-hole susceptibility $\chi_0^{\text{ph}}(\mathbf{q})$ is renormalised to become

$$\chi_{\text{RPA}}^{\text{ph}}(\mathbf{q}) = \frac{\chi_0^{\text{ph}}(\mathbf{q})}{1 - U\chi_0^{\text{ph}}(\mathbf{q})} \quad (2.2)$$

where the Stoner criterion for magnetic instability is given by $U\chi_0^{\text{ph}}(\mathbf{Q}) = 1$, where $\mathbf{Q}$ is the momentum at which χ_0^{ph} is maximal. Within a spin-fluctuation type theory, the system sits close to the transition, $\chi_0^{\text{ph}}(\mathbf{Q})U = 1 - \eta$, with $\eta \ll 1$ and $\chi_{\text{RPA}}^{\text{ph}}(\mathbf{q})$ therefore exhibits strong peaks at certain momenta. The symmetry of the order parameter depends crucially on the position of these maxima. Compared to weak coupling, these finite coupling theories have to deal with several complications. First, the spin fluctuations not only affect the effective interaction, but also single-fermion propagators. Second, one needs to deal with the dissipation of the spin fluctuations by the Fermi liquid through the decay into particle-hole pairs, also called Landau damping. Third, one needs to take into account the competition with magnetic order, since the system sits close to it by construction. Functional renormalisation group [7] calculations were developed to study the competition between these different order parameters. One should also mention spin-fermion models, where the soft spin fluctuations are introduced semi-phenomenologically [8].

In this chapter, we present a weak coupling theory of superconductivity in multi-orbital, spin-orbit coupled materials. In Sect. 2.2, we introduce the model Hamiltonian that will be used throughout this Chapter, the multi-orbital Hubbard model. In Sect. 2.3, we show how a spin-orbit coupled system can be understood in terms of pseudo-spin if it is time-reversal and parity invariant. We introduce a pseudo-spin $\vec{d}$ vector to describe a pseudo-spin triplet superconducting order parameter. In Sect. 2.4, we introduce the susceptibility in the Cooper channel as the quantity giving the response to a small field coupled to the superconducting order parameter. We then give the Feynman rules used to compute this susceptibility perturbatively. In Sect. 2.5, we show that this susceptibility satisfies the Bethe-Salpeter equation, and express the condition of its divergence in terms of the effective interaction. We introduce a pairing matrix whose eigenvalues give T_c and eigenmodes give the order parameter functional forms. In Sect. 2.6, we calculate the effective interaction in perturbation theory in the pseudo-spin singlet and triplet channels. In Sect. 2.7, we use a BCS mean-field Hamiltonian with the order parameters found previously to study the system below T_c . We finish with a conclusion.

2.2 Multi-orbital Hubbard Model

Our starting point will be one of the most studied models for quantum materials, the multi-orbital Hubbard model [9, 10], whose Hamiltonian is

$$\begin{aligned}
 H = H_K + H_I = & \sum_{\mathbf{k}} \sum_{a,a',s,s'} h_{a,s;a',s'}(\mathbf{k}) c_{\mathbf{k},a,s}^\dagger c_{\mathbf{k},a',s'} \\
 & + \frac{1}{4} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} \sum_{a_i,s_i} V_{a_1,s_1,a_2,s_2;a_3,s_3,a_4,s_4} c_{\mathbf{k}_1,a_1,s_1}^\dagger c_{\mathbf{k}_2,a_2,s_2}^\dagger c_{\mathbf{k}_3,a_3,s_3} c_{\mathbf{k}_4,a_4,s_4}
 \end{aligned} \tag{2.3}$$

where a is an index that runs over N_b different atomic orbitals in each unit cell, $s = \pm 1$ is the spin index and $\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}$ stands for a sum over $\mathbf{k}_1$, $\mathbf{k}_2$ and $\mathbf{k}_3$ over the full Brillouin zone, while $\mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$. Many-electron states are generated by acting with creation operators $c_{\mathbf{k},a,s}^\dagger$ on the vacuum state $|\Omega\rangle$. These operators are the creation operators of plane wave states, $|\mathbf{k}, a, s\rangle = c_{\mathbf{k},a,s}^\dagger |\Omega\rangle$ with:

$$c_{\mathbf{k},a,s}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{r},a,s}^\dagger \tag{2.4}$$

where $\mathbf{r}$ are the sites of a given Bravais lattice and N is the total number of sites. We assume a Bravais lattice to simplify notations but it is not a restriction of the scheme. Creation and annihilation operators obey fermionic statistics:

$$\begin{aligned}
\{c_i, c_j\} &= 0 \\
\{c_i^\dagger, c_j^\dagger\} &= 0 \\
\{c_i, c_j^\dagger\} &= \delta_{i,j}
\end{aligned} \tag{2.5}$$

where $\{a, b\} = ab + ba$ and where i, j are generic indices and $\delta_{i,j}$ is the Kronecker delta.

H_K is the single-particle part of the Hamiltonian. It describes the hopping of electrons between different sites, the chemical potential, and the spin-orbit coupling. We are working in the grand-canonical ensemble, where the number of electrons is not fixed, and the expression given in Eq. 2.3 gives $H = \mathcal{H} - \mu N$, where $\mathcal{H}$ is strictly speaking the Hamiltonian, N is the total number of electrons and μ is the chemical potential. In this ensemble, at a temperature $T = \beta^{-1}$ (we take the Boltzmann constant k_B to be 1), the expectation value of a given operator $\mathcal{O}$ is given by

$$\langle \mathcal{O} \rangle = \frac{\text{Tr}[\mathcal{O}e^{-\beta H}]}{\text{Tr}[e^{-\beta H}]} \tag{2.6}$$

For the sake of simplicity, in the following, we will always refer to H as the Hamiltonian, even though, strictly speaking, $\mathcal{H}$ is the Hamiltonian.

H_I describes the repulsion between electrons. Note that $V_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4}$ does not depend on momenta, as we will always consider on-site interactions in the following. Note also that for a given unordered set of indices $(\mathbf{k}_1, a_1, s_1; \mathbf{k}_2, a_2, s_2)$ for creation operators and $(\mathbf{k}_3, a_3, s_3; \mathbf{k}_4, a_4, s_4)$ for annihilation operators, there are always four terms in the sum for H_I that will match this set. The four different terms correspond to permutation of the indices between $\mathbf{k}_1, a_1, s_1$ and $\mathbf{k}_2, a_2, s_2$, and between $\mathbf{k}_3, a_3, s_3$ and $\mathbf{k}_4, a_4, s_4$. We choose a parametrization of the interaction such that these four terms are equal, which, given the anticommutation relation of fermionic operators, is ensured by imposing

$$\begin{aligned}
V_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4} &= V_{a_2, s_2, a_1, s_1; a_4, s_4, a_3, s_3} \\
&= -V_{a_1, s_1, a_2, s_2; a_4, s_4, a_3, s_3} \\
&= -V_{a_2, s_2, a_1, s_1; a_3, s_3, a_4, s_4}
\end{aligned} \tag{2.7}$$

In the following, we will sometimes use t to refer to the energy scale of the hoppings and U to the energy scale of the interaction. We therefore have

$$\begin{aligned}
h_{a, s; a', s'}(\mathbf{k}) &= t \tilde{h}_{a, s; a', s'}(\mathbf{k}) \\
V_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4} &= U \tilde{V}_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4}
\end{aligned} \tag{2.8}$$

where $\tilde{h}_{a, s; a', s'}(\mathbf{k})$ and $\tilde{V}_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4}$ are dimensionless quantities defined such that the largest hopping amplitude in $\tilde{h}_{a, s; a', s'}(\mathbf{k})$ is 1 and such that the largest interaction matrix element in $\tilde{V}_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4}$ is 1.

While the discussion given in this Chapter is very general, we will often give the example of the single-orbital Hubbard model on a D -dimensional hypercubic lattice for illustrative purposes. This model is given by

$$H = \sum_{\mathbf{k}} \xi(\mathbf{k}) \sum_s c_{\mathbf{k},s}^\dagger c_{\mathbf{k},s} + U \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} c_{\mathbf{k}_1,\uparrow}^\dagger c_{\mathbf{k}_2,\downarrow}^\dagger c_{\mathbf{k}_3,\downarrow} c_{\mathbf{k}_4,\uparrow} \quad (2.9)$$

It is easily checked that this corresponds to $V_{s_1,s_2;s_3,s_4} = U \delta_{s_1,-s_2} \delta_{s_3,-s_4} (\delta_{s_2,s_3} - \delta_{s_2,s_4})$ in the parametrization of Eq. 2.3. The single-particle energy ξ is obtained by diagonalizing the hoppings. For example, for nearest-neighbor hopping and $D = 2$ (square lattice), one has

$$H_K = -t \left(\sum_{\mathbf{r}} c_{\mathbf{r}+\hat{x}}^\dagger c_{\mathbf{r}} + c_{\mathbf{r}+\hat{y}}^\dagger c_{\mathbf{r}} + \text{h.c.} \right) - \mu \sum_{\mathbf{r}} c_{\mathbf{r}}^\dagger c_{\mathbf{r}} \quad (2.10)$$

where $\mathbf{r}$ runs over all sites, $\hat{x}$ and $\hat{y}$ are the unit vectors (the lattice constant is taken to be 1), t is the tunnelling amplitude and μ is the chemical potential. This leads to $\xi(\mathbf{k}) = -2t(\cos(k_x) + \cos(k_y)) - \mu$.

In this chapter, we start from the Hubbard Hamiltonian and present a weak coupling calculation of the superconducting instability arising in this model. In order to relate the so-obtained results to a given material, one should of course first establish the relevance of the Hubbard model to the material. This will be done in details in the next chapter for the case of Sr_2RuO_4 , but we can already give a short justification. As a starting point to study a given material, one can use an Hartree-Fock type calculation to obtain a band structure that incorporates interactions between electrons at a mean-field level [9]. If this band structure happens to have conduction bands with a small bandwidth compared to the typical size of the effective interactions between electrons populating this band, the correlations arising from the interactions are expected to be too important to be neglected in a mean-field calculation. The Hubbard model is then used as an effective model where a tight-binding approximation is used to reproduce the narrow band and an on-site interaction is used to reproduce the effective interaction between electrons of this band. Compared to the bare Coulomb repulsion, this interaction is screened by the valence and conduction bands and therefore decays exponentially with distance. Typically, this screened interaction is sizeable only over a few lattice sites, and the approximation of keeping only the on-site part of the interaction is then justified.

2.3 Pseudo-spin Basis

We first diagonalize the single-particle Hamiltonian H_K . Without spin-orbit coupling, this Hamiltonian is diagonal in spin space, and each of the two spin species has the same hoppings, $h_{a,s;a',s'}(\mathbf{k}) = h_{a,a'}(\mathbf{k})\delta_{s,s'}$. After diagonalization, one obtains

N_b doubly-degenerate bands, where the degeneracy comes from the spin degree of freedom, $H_K = \sum_{\mathbf{k}, \alpha} \xi_\alpha(\mathbf{k}) (c_{\mathbf{k}, \alpha, \uparrow}^\dagger c_{\mathbf{k}, \alpha, \uparrow} + c_{\mathbf{k}, \alpha, \downarrow}^\dagger c_{\mathbf{k}, \alpha, \downarrow})$, where α is the band index.

While the discussion so far has been fairly general, the impact of spin-orbit coupling can vary a lot depending on the materials. The type of systems considered in this thesis are such that the relevant dynamics happens in partially filled bands of the d orbitals of some transition metal element, like Copper ($3d$), Iron ($3d$), Ruthenium ($4d$), Iridium ($5d$), ... In these compounds, the transition metal is typically surrounded by so-called ligand ions, like Oxygen in the case Sr_2RuO_4 or Selenium in the case of Iron Selenide, FeSe . In the perovskite structure of Sr_2RuO_4 , the Oxygen ions form an octahedron around Ruthenium atoms (see Fig. 1.1). Since we are only interested in the bands crossing the Fermi level, our tight-binding model will only include the atomic orbitals that have a sizeable contribution at the Fermi level, and the spin-orbit coupling will thus only be taken into account for these orbitals.

Starting from the idealized case of an isolated transition metal ion, two effects are to be taken into account: the effect of the ligand ions (i.e. the so-called crystal field), and spin-orbit coupling. The terms arising in the Hamiltonian from these two effects do not commute and one typically resorts to the following approximation: (1) diagonalize the largest of the two terms, (2) treat the second term in perturbation theory to split the remaining degeneracies. In this thesis, we will treat the case of a dominant crystal field, as it is the case relevant for Sr_2RuO_4 . Note that the case of a dominant spin-orbit coupling is also of interest since it occurs for transition metals atoms with a $5d$ shell, like Iridium. Iridates were shown to exhibit a large range of interesting phases [11].

First, one should treat the effect of the ligand ions. This so-called crystal field breaks rotational invariance down to the discrete symmetry group of the configuration of ligand ions. The crystal field generates a splitting between different atomic orbitals consistently with this reduced symmetry. In the case of Sr_2RuO_4 , this crystal field splits the e_g doublet ($d_{x^2-y^2}$ and d_{z^2}) from the t_{2g} triplet (d_{xz} , d_{yz} and d_{xy}), and only the latter orbitals are relevant close to the Fermi level. The e_g orbitals point towards the vertices of the octahedra, i.e. the position of the Oxygen atoms, while the t_{2g} orbitals point towards the edges of the octahedra. The t_{2g} orbitals are therefore less hybridised with the Oxygen p orbitals.

Second, one should add the effect of the spin-orbit interaction. For an isolated atom with full rotational invariance, this term would be written as

$$H_{\text{SOC}}^{\text{atom}} = \eta \vec{L} \cdot \vec{S} \quad (2.11)$$

where η is the SOC constant which, within our formalism, is better kept as an adjustable phenomenological parameter, $\vec{L}$ is the orbital angular momentum and $\vec{S}$ is the spin angular momentum. In contrast, in the presence of a strong crystal field, the spin-orbit coupling is treated perturbatively and diagonalized within the subspace of the orbitals relevant close to the Fermi level. When the crystal field is the dominating effect, the most convenient basis of atomic orbitals is the one of real atomic orbitals, like d_{xz} , d_{yz} and d_{xy} , as opposed to L_z eigenvectors. In the following, we will use a as

a generic index for these real orbitals used in the tight-binding Hamiltonian. Finally, summing over all atoms, the SOC term is inserted in the tight-binding model as

$$H_{\text{SOC}} = \eta \sum_i P \vec{L}_i \cdot \vec{S}_i P \quad (2.12)$$

where i is the atom index and P is the projector to the subspace of real atomic orbitals relevant close to the Fermi level, which are indexed by $a = 1, \dots, N_b$.

The single-particle Hamiltonian H_K can now be written as $H_K = H_{\text{Hop}} + H_{\text{SOC}}$ where H_{Hop} gives both intra- and inter-orbital hopping terms. While this Hamiltonian does not have a spin $SU(2)$ symmetry because of H_{SOC} , it still has time-reversal symmetry and parity. Thanks to these two symmetries, the bands are still doubly-degenerate, as we now show. A time-reversal symmetric system is a system that is invariant under a transformation where the time t is replaced by $-t$. An inversion (or parity) symmetric system is a system that is invariant under a transformation where the spatial coordinates (x, y, z) are replaced by $(-x, -y, -z)$. More specifically, the time-reversal operator is defined as the anti-unitary operator $\mathcal{T} = T\mathcal{K}$, where $\mathcal{K}$ is the complex conjugation operator and T is given by

$$T |\mathbf{k}, a, s\rangle = s |-\mathbf{k}, a, -s\rangle. \quad (2.13)$$

The inversion operator is defined as

$$\mathcal{P} |\mathbf{k}, a, s\rangle = |-\mathbf{k}, a, s\rangle \quad (2.14)$$

where, in order to simplify notations, we have assumed that all a orbitals are even under parity, which is the case for the d orbitals we will be interested in. A system is time-reversal symmetric if its Hamiltonian satisfies $\mathcal{T}H\mathcal{T}^{-1} = H$ and inversion symmetric if $\mathcal{P}H\mathcal{P}^{-1} = H$. Say we have a single-particle eigenvector of H_K given by $|\mathbf{k}, \alpha\rangle = \sum_{a,s} u_{a,s}^\alpha |\mathbf{k}, a, s\rangle$. By time-reversal symmetry and inversion symmetry, we know that $\mathcal{P}\mathcal{T} |\mathbf{k}, \alpha\rangle$ is also an eigenvector with the same energy and the same momentum. It therefore only remains to show that these two states are not the same, which is easily shown by showing that their overlap vanishes: $\langle \mathbf{k}, \alpha | \mathcal{P}\mathcal{T} |\mathbf{k}, \alpha\rangle = \sum_{a,s} u_{a,s}^* u_{a,-s}^* s = \sum_a (u_{a,\uparrow}^* u_{a,\downarrow}^* - u_{a,\downarrow}^* u_{a,\uparrow}^*) = 0$.

Since each band is doubly degenerate, it will be useful to define a pseudo-spin $\sigma = \pm 1$ to index these two degenerate states. After diagonalization, the Hamiltonian reads

$$H_K = \sum_\alpha \sum_{\mathbf{k}} \xi_{\mathbf{k},\alpha} (c_{\mathbf{k},\alpha,\sigma=+1}^\dagger c_{\mathbf{k},\alpha,\sigma=+1} + c_{\mathbf{k},\alpha,\sigma=-1}^\dagger c_{\mathbf{k},\alpha,\sigma=-1}). \quad (2.15)$$

with

$$c_{\mathbf{k},\alpha,\sigma}^\dagger = \sum_{a,s} u_{a,s}^{\alpha,\sigma}(\mathbf{k}) c_{\mathbf{k},a,s}^\dagger. \quad (2.16)$$

We can now rewrite the entire Hamiltonian given in Eq. 2.3 in the band and pseudo-spin basis:

$$H = H_K + H_I = \sum_{\alpha} \sum_{\mathbf{k}} \xi_{\mathbf{k},\alpha} (c_{\mathbf{k},\alpha,\sigma=+1}^{\dagger} c_{\mathbf{k},\alpha,\sigma=+1} + c_{\mathbf{k},\alpha,\sigma=-1}^{\dagger} c_{\mathbf{k},\alpha,\sigma=-1}) + \frac{1}{4} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} \sum_{\alpha_i, \sigma_i} V_{\mathbf{k}_1, \alpha_1, \sigma_1, \mathbf{k}_2, \alpha_2, \sigma_2; \mathbf{k}_3, \alpha_3, \sigma_3, \mathbf{k}_4, \alpha_4, \sigma_4} c_{\mathbf{k}_1, \alpha_1, \sigma_1}^{\dagger} c_{\mathbf{k}_2, \alpha_2, \sigma_2}^{\dagger} c_{\mathbf{k}_3, \alpha_3, \sigma_3} c_{\mathbf{k}_4, \alpha_4, \sigma_4} \quad (2.17)$$

where

$$V_{\mathbf{k}_1, \alpha_1, \sigma_1, \mathbf{k}_2, \alpha_2, \sigma_2; \mathbf{k}_3, \alpha_3, \sigma_3, \mathbf{k}_4, \alpha_4, \sigma_4} = \sum_{a_i, s_i} V_{a_1, s_1, a_2, s_2; a_3, s_3, a_4, s_4} u_{a_1, s_1}^{\alpha_1, \sigma_1}(\mathbf{k}_1) u_{a_2, s_2}^{\alpha_2, \sigma_2}(\mathbf{k}_2) (u_{a_3, s_3}^{\alpha_3, \sigma_3}(\mathbf{k}_3))^* (u_{a_4, s_4}^{\alpha_4, \sigma_4}(\mathbf{k}_4))^* \quad (2.18)$$

From Eq. 2.7, it is easy to see that

$$\begin{aligned} V_{\mathbf{k}_1, \alpha_1, \sigma_1, \mathbf{k}_2, \alpha_2, \sigma_2; \mathbf{k}_3, \alpha_3, \sigma_3, \mathbf{k}_4, \alpha_4, \sigma_4} &= V_{\mathbf{k}_2, \alpha_2, \sigma_2, \mathbf{k}_1, \alpha_1, \sigma_1; \mathbf{k}_4, \alpha_4, \sigma_4, \mathbf{k}_3, \alpha_3, \sigma_3} \\ &= -V_{\mathbf{k}_2, \alpha_2, \sigma_2, \mathbf{k}_1, \alpha_1, \sigma_1; \mathbf{k}_3, \alpha_3, \sigma_3, \mathbf{k}_4, \alpha_4, \sigma_4} \\ &= -V_{\mathbf{k}_1, \alpha_1, \sigma_1, \mathbf{k}_2, \alpha_2, \sigma_2; \mathbf{k}_4, \alpha_4, \sigma_4, \mathbf{k}_3, \alpha_3, \sigma_3} \end{aligned} \quad (2.19)$$

2.3.1 Pseudo-spin and Crystal Symmetries

One needs to choose a convention to decide which state is $\sigma = +1$ and which one is $\sigma = -1$, and this decision should be made at every $\mathbf{k}$ point. While this is purely a matter of convention, some choices are more advantageous if one wants to use similar tools and notations that exist in the case of $SU(2)$ -invariant systems.

In analogy with the $SU(2)$ -invariant case, it is advantageous to choose the pseudo-spin basis so that $T|\mathbf{k}, \alpha, \sigma\rangle = \sigma|-\mathbf{k}, \alpha, -\sigma\rangle$ and $\mathcal{P}|\mathbf{k}, \alpha, \sigma\rangle = |-\mathbf{k}, \alpha, \sigma\rangle$. Furthermore, besides $\mathcal{P}$, the point group of the crystal can also include discrete rotational symmetries. With the inclusion of spin-orbit coupling, these rotations should act simultaneously in real space and in spin space in order to commute with the Hamiltonian. For each element of the point group, one obtains an element of the so-called double group [12] by performing it in both real and spin space. A given element of the double group $\mathcal{R}$ acts in the following way:

$$\mathcal{R}|\mathbf{k}, a, s\rangle = \mathcal{R}^O \mathcal{R}^S |\mathbf{k}, a, s\rangle = R_{a,a'}^O R_{s,s'}^S |\mathcal{R}\mathbf{k}, a', s'\rangle \quad (2.20)$$

where $R_{a,a'}^O$ is the rotation matrix in the space of atomic orbitals, $R_{s,s'}^S$ is the rotation matrix in spin space, $\mathcal{R}\mathbf{k}$ is the image of the vector $\mathbf{k}$ under the rotation $\mathcal{R}$ and where the summation over repeated indices is implied. If $\mathcal{R}$ is a rotation of angle θ and axis $\hat{n}$, one has $\mathcal{R}^O = e^{-i\theta\hat{n}\cdot\vec{L}}$ and $\mathcal{R}^S = e^{-i\theta\hat{n}\cdot\vec{S}}$ ($\hbar$ is set to one everywhere in this

thesis). From Eq. 2.14, we find that for the parity transformation, i.e. $\mathcal{R} = \mathcal{P}$, one has $\mathcal{R}^O = \mathbb{1}$, $\mathcal{R}^S = \mathbb{1}$ and of course $\mathcal{R}\mathbf{k} = -\mathbf{k}$.

In analogy with the case without spin-orbit coupling, it is advantageous to choose the pseudo-spin basis so that the following relation holds:

$$\mathcal{R} |\mathbf{k}, \alpha, \sigma\rangle = R_{\sigma, \sigma'}^S |\mathcal{R}\mathbf{k}, \alpha, \sigma'\rangle. \quad (2.21)$$

In this way, under discrete rotations of the double group, each band behaves as if it were a single (s -wave) orbital, and the pseudo-spin behaves in the same way as a regular spin would. The advantage of this basis choice is that the pseudo-spin triplet superconducting order parameter $\vec{d}$ will transform like a vector under the double group, and the pseudo-spin singlet order parameter will transform like a scalar. This will be explained in the next Section.

One simple way to achieve this is to proceed as follows. First, for each $\mathbf{k}$ in the irreducible Brillouin zone (the smallest subset of the BZ such that any $\mathbf{k}$ can be folded back to it by an element of the point group) and for each band α , pick an arbitrary eigenvector and assign it the value of $\sigma = +1$, i.e. declare it to be $|\mathbf{k}, \alpha, \sigma = +1\rangle$. Once this is done, $|\mathbf{k}, \alpha, \sigma = -1\rangle$ is defined up to a phase, which we fix by posing $|\mathbf{k}, \alpha, \sigma = -1\rangle \equiv \mathcal{TP} |\mathbf{k}, \alpha, \sigma = +1\rangle$. Second, for every $\mathbf{k}$ point outside the irreducible BZ, define the basis as

$$|\mathbf{k}, \alpha, \sigma\rangle = \left((R^S)^{-1} \right)_{\sigma, \sigma'} \mathcal{R} |\mathcal{R}^{-1}\mathbf{k}, \alpha, \sigma'\rangle \quad (2.22)$$

where $\mathcal{R}^{-1}\mathbf{k}$ is in the irreducible BZ.

Note that, due to the double covering of $SO(3)$ by $SU(2)$, elements of the double group that correspond to 2π rotations have $R^S = -\mathbb{1}$ and are therefore not the identity element. The solutions for finding $\mathcal{R}$ such that $\mathcal{R}^{-1}\mathbf{k}$ is in the irreducible BZ are therefore only obtained modulo these 2π rotations. This simply leads to a sign ambiguity in the above scheme, which can be easily fixed by restricting $\mathcal{R}$ in Eq. 2.22 to rotations of angles in the range $[0, 2\pi[$. This arbitrary choice of sign will be inconsequential in the following, since we will only be interested in the transformation of Cooper pair operators, for which two electrons are transformed at the same time and the -1 factors would therefore cancel.

2.3.2 Superconducting Order Parameter in Pseudo-Spin Basis

In the next section, we will introduce the superconducting order parameter as the non-zero expectation value of Cooper pair operators of the form

$$\phi_{\sigma, \sigma'}(\mathbf{k}, \alpha) \equiv c_{\mathbf{k}, \alpha, \sigma} c_{-\mathbf{k}, \alpha, \sigma'} \quad (2.23)$$

In the single orbital $SU(2)$ -invariant case, Balian and Werthamer [13] introduced the following parametrization of the spin degrees of freedom of the Cooper pair:

$$\begin{pmatrix} \phi_{\uparrow\uparrow}(\mathbf{k}) & \phi_{\uparrow\downarrow}(\mathbf{k}) \\ \phi_{\downarrow\uparrow}(\mathbf{k}) & \phi_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\phi_{d_x}(\mathbf{k}) + i\phi_{d_y}(\mathbf{k}) & \phi_{d_z}(\mathbf{k}) + \phi_{d_0}(\mathbf{k}) \\ \phi_{d_z}(\mathbf{k}) - \phi_{d_0}(\mathbf{k}) & \phi_{d_x}(\mathbf{k}) + i\phi_{d_y}(\mathbf{k}) \end{pmatrix}, \quad (2.24)$$

where $\phi_{s,s'}(\mathbf{k}) = c_{\mathbf{k},s}c_{-\mathbf{k},s'}$. This parametrization is advantageous because the spin singlet (resp. triplet) order parameter ϕ_{d_0} (resp. $\phi_{\vec{d}}$) is a scalar (resp. vector) under any spin-space rotation $\mathcal{R}^S$:

$$\begin{aligned} \mathcal{R}^S \phi_{d_0}(\mathbf{k})(\mathcal{R}^S)^{-1} &= \phi_{d_0}(\mathbf{k}) \\ \mathcal{R}^S \phi_{\vec{d}}(\mathbf{k})(\mathcal{R}^S)^{-1} &= \phi_{\mathcal{R}\vec{d}}(\mathbf{k}). \end{aligned} \quad (2.25)$$

In analogy with the $SU(2)$ -invariant case, we rearrange the pseudo-spin degrees of freedom in a singlet ϕ_{d_0} and a triplet $\phi_{\vec{d}}$:

$$\begin{pmatrix} \phi_{++} & \phi_{+-} \\ \phi_{-+} & \phi_{--} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\phi_{d_x} + i\phi_{d_y} & \phi_{d_z} + \phi_{d_0} \\ \phi_{d_z} - \phi_{d_0} & \phi_{d_x} + i\phi_{d_y} \end{pmatrix}, \quad (2.26)$$

where we have left the indices $\mathbf{k}$, α implicit. Now, using the property of the pseudo-spin basis given in Eq. 2.21, one can check that the pseudo-spin order parameters behave in the appropriate way under any element of the double group $\mathcal{R}$:

$$\begin{aligned} \mathcal{R}\phi_{d_0}(\mathbf{k}, \alpha)\mathcal{R}^{-1} &= \phi_{d_0}(\mathcal{R}\mathbf{k}, \alpha) \\ \mathcal{R}\phi_{\vec{d}}(\mathbf{k}, \alpha)\mathcal{R}^{-1} &= \phi_{\mathcal{R}\vec{d}}(\mathcal{R}\mathbf{k}, \alpha) \end{aligned} \quad (2.27)$$

This means that, when classifying the different possible pseudo-spin order parameters, we can use the irreducible representations of the point group.

2.4 Linear Response

In order to study the onset of superconductivity, let us compute the susceptibility of the system to the appearance of a superconducting order parameter within linear response theory. The divergence of this quantity will mark the onset of superconductivity. The order parameter is given by the non-zero expectation value of the Cooper pair creation operator $\phi_{\mathbf{k},\alpha,\sigma,\sigma'}^\dagger \equiv c_{\mathbf{k},\alpha,\sigma}^\dagger c_{-\mathbf{k},\alpha,\sigma'}^\dagger$.

In general, one should consider the possibility of other order parameters, including Cooper pairing at finite momentum and frequencies, and spin-density wave (SDW) or charge-density wave (CDW) order. Instead, in the weak coupling limit, it was shown (see for example Ref. [5]) that, except for a few exceptions that will be discussed below, the only instability is the zero-frequency, zero-momentum Cooper pairing and it is therefore sufficient to consider only this order parameter. Note that we

only considered pairing between electrons of the same band. This is justified if the superconducting gap scale is much smaller than the energy separation between the different bands close to the Fermi level, which is generically true in the $U/t \rightarrow 0$ limit.

A non-zero expectation value of ϕ breaks the $U(1)$ symmetry $c_{\mathbf{k},\alpha,\sigma,\sigma'} \rightarrow c_{\mathbf{k},\alpha,\sigma,\sigma'} e^{i\theta}$ associated with the conservation of the total number (or charge) of electrons. As such, if we naively compute a thermal expectation value of the type $\text{Tr}[e^{-\beta H} \phi_{\mathbf{k},\alpha,\sigma,\sigma'}] / \text{Tr}[e^{-\beta H}]$, it would always be zero by symmetry. Instead, one can imagine applying a vanishingly small field coupled to the superconducting order parameter, calculate the thermal average with that small field, and then take the field to zero at the end. With this small perturbation, the Hamiltonian becomes $H + H_J$ with

$$H_J = \sum_{\mathbf{k}} J_{\mathbf{k},\alpha,\sigma,\sigma'} \phi_{\mathbf{k},\alpha,\sigma,\sigma'} + h.c. \quad (2.28)$$

where $J_{\mathbf{k},\alpha,\sigma,\sigma'}$ is some arbitrary complex function much smaller than the energy scale set by H . As a reminder, $H = H_K + H_I$ is the unperturbed Hamiltonian and was given previously. We want to compute the expectation value of ϕ for the perturbed system:

$$\langle \phi_{\mathbf{k},\alpha,\sigma,\sigma'} \rangle = \frac{\text{Tr}[e^{-\beta(H+H_J)} \phi_{\mathbf{k},\alpha,\sigma,\sigma'}]}{\text{Tr}[e^{-\beta(H+H_J)}]} \quad (2.29)$$

2.4.1 Field Theory Formalism

It is now advantageous to use the coherent state fermionic field theory derived from the Hamiltonian $H + H_J$ [5]:

$$\begin{aligned} S + S_J &= S_K + S_I + S_J \\ &= \frac{1}{\beta} \sum_{\mathbf{k},!,\alpha} (i\omega - \xi_{\mathbf{k},\alpha}) \bar{\Psi}_{\mathbf{k},\omega,\alpha,\sigma} \Psi_{\mathbf{k},\omega,\alpha,\sigma} \\ &\quad - \frac{1}{4} \frac{1}{\beta^3} \sum_{\mathbf{k}_i, \omega_i, \alpha_i, \sigma_i} V_{\mathbf{k}_1, \alpha_1, \sigma_1, \mathbf{k}_2, \alpha_2, \sigma_2; \mathbf{k}_3, \alpha_3, \sigma_3, \mathbf{k}_4, \alpha_4, \sigma_4} \bar{\Psi}_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1} \bar{\Psi}_{\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2} \\ &\quad \Psi_{\mathbf{k}_3, \omega_3, \alpha_3, \sigma_3} \Psi_{\mathbf{k}_4, \omega_4, \alpha_4, \sigma_4} \\ &\quad - \frac{1}{\beta} \sum_{\mathbf{k},!,\alpha,\sigma'} J_{\mathbf{k},\alpha,\sigma,\sigma'} \Psi_{-\mathbf{k}, -\omega, \alpha, \sigma'} \Psi_{\mathbf{k}, \omega, \alpha, \sigma} + (J_{\mathbf{k},\alpha,\sigma,\sigma'})^* \bar{\Psi}_{\mathbf{k}, \omega, \alpha, \sigma} \bar{\Psi}_{-\mathbf{k}, -\omega, \alpha, \sigma'} \end{aligned} \quad (2.30)$$

where $\Psi_{\mathbf{k},\omega,\alpha,\sigma}$ is a Grassman number and has the dimension of the inverse of an energy, the sum over ω_i is such that $\omega_1 + \omega_2 = \omega_3 + \omega_4$ and the sum over $\mathbf{k}_i$ is such that $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$ modulo a reciprocal lattice vector. Grassman numbers anticommute with each other, commute with regular numbers, and square to zero [5].

The Matsubara frequencies that are summed over are given by $\omega = \frac{(2n+1)\pi}{\beta}$, with n any integer. In the zero-temperature limit, $\frac{1}{\beta} \sum_{\omega} \rightarrow \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}$. In the thermodynamic limit, $\sum_{\mathbf{k}} \rightarrow \int \frac{d\mathbf{k}}{(2\pi)^D}$ where the integral is over the Brillouin zone and D is the number of spatial dimensions.

For a given operator $\mathcal{O}$, one defines its evolution in imaginary time τ by $\mathcal{O}_{\tau} = e^{(H+H_J)\tau} \mathcal{O} e^{-(H+H_J)\tau}$. If $\mathcal{O}_{\tau}$ is expressed in terms of c_{τ} and $c_{\tau}^{\dagger}$ in a normal-ordered way (i.e. with each creation operator to the left of its annihilation operator), its expectation value is obtained in the field theory formalism by replacing each c ($c^{\dagger}$) by the corresponding Grassman number Ψ ($\bar{\Psi}$). Within this formalism, we can now compute the expectation value given earlier:

$$\begin{aligned} \langle \phi_{\mathbf{k}, \alpha, \sigma, \sigma'} \rangle &= \langle \Psi_{-\mathbf{k}, \tau=0, \alpha, \sigma'} \Psi_{\mathbf{k}, \tau=0, \alpha, \sigma} \rangle_{S+S_J} \\ &= Z^{-1} \int D(\bar{\Psi}, \Psi) e^{S+S_J} \Psi_{-\mathbf{k}, \tau=0, \alpha, \sigma'} \Psi_{\mathbf{k}, \tau=0, \alpha, \sigma} \end{aligned} \quad (2.31)$$

with $Z = \int D(\bar{\Psi}, \Psi) e^{S+S_J}$. We now use the fact that the perturbation H_J is small to write $e^{S_J} \simeq 1 + S_J$, leading to

$$\begin{aligned} \langle \phi_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1} \rangle &\simeq -\frac{1}{\beta} \sum_{\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} (J_{\mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2})^* \\ &\quad \langle \bar{\Psi}_{\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2} \bar{\Psi}_{-\mathbf{k}_2, -\omega_2, \alpha_2, \sigma'_2} \Psi_{-\mathbf{k}_1, \tau=0, \alpha_1, \sigma'_1} \Psi_{\mathbf{k}_1, \tau=0, \alpha_1, \sigma_1} \rangle_S. \end{aligned} \quad (2.32)$$

Using

$$\begin{aligned} \Psi_{\tau} &= \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} \Psi_{\omega} \\ \bar{\Psi}_{\tau} &= \frac{1}{\beta} \sum_{\omega} e^{i\omega\tau} \bar{\Psi}_{\omega}, \end{aligned} \quad (2.33)$$

we can now Fourier transform the two last Grassman variables, leading to

$$\begin{aligned} \langle \phi_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1} \rangle &= -\frac{1}{\beta^3} \sum_{\mathbf{k}_2, \omega_1, \omega_2, \alpha_2, \sigma_2, \sigma'_2} \chi_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2}^{\text{SC}} (J_{\mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2})^* \\ \chi_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2}^{\text{SC}} &= \langle \bar{\Psi}_{\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2} \bar{\Psi}_{-\mathbf{k}_2, -\omega_2, \alpha_2, \sigma'_2} \Psi_{-\mathbf{k}_1, -\omega_1, \alpha_1, \sigma'_1} \Psi_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1} \rangle_S. \end{aligned} \quad (2.34)$$

χ^{SC} is the susceptibility in the Cooper channel, and will be shown to diverge in the thermodynamic limit at a critical temperature T_c . In order to evaluate χ^{SC} , we use a perturbation expansion in the interaction S_I , and we are left with having to evaluate only expectation values with respect to S_K , which can be done by using Wick's theorem since S_K is quadratic. This perturbation theory is best described in terms of Feynman diagrams [14].

The Feynman rules to compute a fermionic correlator are the following. Solid lines are free electron propagators $G_0(\mathbf{k}, \omega, \alpha, \sigma) = (i\omega - \xi_{\mathbf{k},\alpha})^{-1}$. For each fermionic operator $\Psi_{\mathbf{k},\omega,\alpha,\sigma}$ ($\bar{\Psi}_{\mathbf{k},\omega,\alpha,\sigma}$) in the correlator, there is an external leg entering (resp. exiting) the diagram with the same indices $\mathbf{k}, \omega, \alpha, \sigma$. For a given set of external legs, one should sum over all diagrams that connect these external legs. One should not sum over diagrams that include disconnected components that are not linked to the external legs, as these diagrams are cancelled by the denominator in the definition of the expectation value.

A vertex is the association of two incoming and two outgoing fermionic propagators linked by a dashed line, as shown in Fig. 2.4. Momenta and Matsubara frequencies are conserved at each vertex. Thanks to this property, for a given diagram, all sums over internal momenta can be performed readily, except for n_{loop} of them, where n_{loop} is the number of loops in the diagram. Each connected component of the diagram has an overall factor given by $\beta \delta_{\sum_i \omega_i} \delta_{\sum_i \mathbf{k}_i}$, where $\omega_i, \mathbf{k}_i$ are the external frequencies and momenta of that connected component. For each internal propagator, one should sum over its α, σ indices. For each fermionic loop, the diagram picks up a minus sign. A fermionic loop is a loop formed by electron propagators.

The factor of $\frac{1}{4} = \frac{1}{2!2!}$ in the action in front of $-V_{\mathbf{k}_1,\alpha_1,\sigma_1,\mathbf{k}_2,\alpha_2,\sigma_2;\mathbf{k}_3,\alpha_3,\sigma_3,\mathbf{k}_4,\alpha_4,\sigma_4}$ (abbreviated as $-V_{1,2;3,4}$ in the following) takes care of the 4 possible leg permutations of a given vertex ($1 \leftrightarrow 2$ and $3 \leftrightarrow 4$), which all give the same contribution. Two diagrams that only differ by such a permutation are called equivalent. One can therefore sum only over one example diagram in each equivalence class and use a factor of $-V_{1,2;3,4}$ for each vertex. This is correct as long as there are 4^v diagrams in each equivalence class, where v is the number of vertices. In certain equivalence classes, two or more of their fermionic legs can be permuted without changing the diagram. In that case, the number of diagrams is therefore smaller, say $4^v/m$. One should then divide the contribution from this equivalence class by m , which is called the symmetry factor [14].

We are only interested in the divergent part of χ^{SC} , which will arise from the connected part of the expectation value, defined by

$$\begin{aligned} \chi_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1,\sigma'_1;\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2,\sigma'_2}^{\text{SC},c} &= \langle \bar{\Psi}_{\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2} \bar{\Psi}_{-\mathbf{k}_2,-\omega_2,\alpha_2,\sigma'_2} \Psi_{-\mathbf{k}_1,-\omega_1,\alpha_1,\sigma'_1} \Psi_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1} \rangle_S \\ &\quad - \langle \bar{\Psi}_{-\mathbf{k}_2,-\omega_2,\alpha_2,\sigma'_2} \Psi_{-\mathbf{k}_1,-\omega_1,\alpha_1,\sigma'_1} \rangle_S \langle \bar{\Psi}_{\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2} \Psi_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1} \rangle_S \\ &\quad + \langle \bar{\Psi}_{-\mathbf{k}_2,-\omega_2,\alpha_2,\sigma'_2} \Psi_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1} \rangle_S \langle \bar{\Psi}_{\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2} \Psi_{-\mathbf{k}_1,-\omega_1,\alpha_1,\sigma'_1} \rangle_S \end{aligned} \quad (2.35)$$

Since all the diagrams contributing to $\chi^{\text{SC},c}$ will be proportional to $\beta \delta_{\sum_i \omega_i} \delta_{\sum_i \mathbf{k}_i}$ times the four external propagators, we now define

$$\begin{aligned} -\mathcal{V}_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1,\sigma'_1;\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2,\sigma'_2} &\equiv \frac{1}{2} \beta^{-1} (i\omega_1 - \xi_1) (-i\omega_1 - \xi_1) (i\omega_2 - \xi_2) (-i\omega_2 - \xi_2) \\ &\quad \chi_{\mathbf{k}_1,\omega_1,\alpha_1,\sigma_1,\sigma'_1;\mathbf{k}_2,\omega_2,\alpha_2,\sigma_2,\sigma'_2}^{\text{SC},c} \end{aligned} \quad (2.36)$$

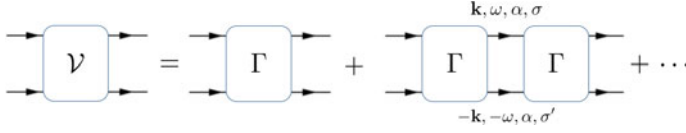


Fig. 2.1 Infinite sum of ladder diagrams

with $\xi_1 = \xi_{\mathbf{k}_1, \alpha_1} = \xi_{-\mathbf{k}_1, \alpha_1}$ and $\xi_2 = \xi_{\mathbf{k}_2, \alpha_2} = \xi_{-\mathbf{k}_2, \alpha_2}$. The minus sign in front is a useful convention so that a negative value of $\mathcal{V}$ indicates attraction, while a positive value indicates repulsion. The factor of $\frac{1}{2}$ is a convenient convention whose usefulness will become clear later (Fig. 2.1).

2.5 Bethe-Salpeter Equation

Based on its previous definition, one finds that $-\mathcal{V}_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2}$ is given by the sum of all connected diagrams with two outgoing external legs ($\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2$ and $-\mathbf{k}_2, -\omega_2, \alpha_2, \sigma'_2$) and two incoming external legs ($\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1$ and $-\mathbf{k}_1, -\omega_1, \alpha_1, \sigma'_1$), where the external propagators and delta functions are stripped off, and where an overall factor of $\frac{1}{2}$ is added (see Fig. 2.2). In order to calculate this, it is advantageous to define $-\Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2}$ in the exact same way, except that only two-particle irreducible (2PI) diagrams are kept (see Fig. 2.3). A 2-particle irreducible diagram is a connected diagram that cannot be split into two admissible diagrams by cutting any two internal propagators. Γ is also called the irreducible vertex and gives the effective interaction between electrons.

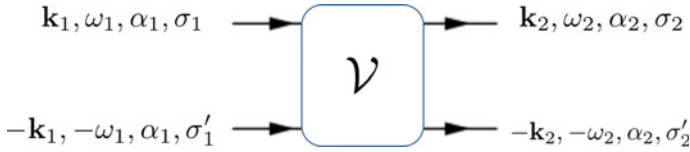


Fig. 2.2 Effective vertex in the Cooper channel, given by the sum of all diagrams with the four external legs represented on the figure, and with certain prefactors defined in the text

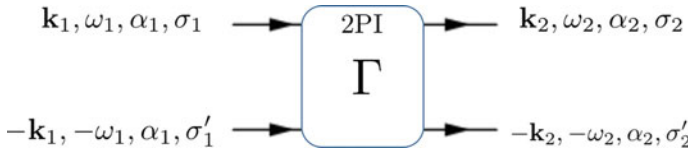


Fig. 2.3 Γ is defined in the same way as $\mathcal{V}$, except that only 2-particle irreducible diagrams are summed over

As a function of Γ , the total susceptibility is given as an infinite sum of ladders, as shown in Fig. 2.1:

$$\begin{aligned} -\mathcal{V} &= -\Gamma + \Gamma \diamond \mathcal{G}^0 \diamond \Gamma - \Gamma \diamond \mathcal{G}^0 \diamond \Gamma \diamond \mathcal{G}^0 \diamond \Gamma + \dots \\ &= -\Gamma + \Gamma \diamond \mathcal{G}^0 \diamond \mathcal{V} \end{aligned} \quad (2.37)$$

where

$$(A \diamond B)_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} = \frac{1}{\beta} \sum_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'} A_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}, \omega, \alpha, \sigma, \sigma'} B_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} \quad (2.38)$$

and

$$\mathcal{G}_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2}^0 = \beta \delta_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} (i\omega_1 - \xi_{\mathbf{k}_1, \alpha_1})^{-1} (-i\omega_1 - \xi_{-\mathbf{k}_1, \alpha_1})^{-1}. \quad (2.39)$$

Combining these definitions, one finds

$$\begin{aligned} (\Gamma \diamond \mathcal{G}^0 \diamond \Gamma)_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} &= \\ \frac{1}{\beta} \sum_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'} (i\omega - \xi_{\mathbf{k}, \alpha})^{-1} (-i\omega - \xi_{-\mathbf{k}, \alpha})^{-1} \Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}, \omega, \alpha, \sigma, \sigma'} \Gamma_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} \end{aligned} \quad (2.40)$$

Equation 2.37 is the Bethe-Salpeter equation [15]. Several comments are in order at this point. Two approximations were made. First, we used free propagators instead of renormalized ones. This is justified in the weak coupling limit by the fact that the use of renormalized propagators would only lead to subdominant corrections in U/t [16]. Second, we did not allow for the pair of internal propagators with opposite momenta and frequencies linking two consecutive Γ blocks to be on different bands. The sum over internal momenta and frequencies for each such pair leads to a logarithmically diverging contribution that is responsible for the pairing instability. This diverging contribution only arises in the case where the two propagators in the pair have the same energy, which forces them to be on the same band due to inversion symmetry. This is why we have left out diagrams where the two rails of the ladder are on different bands, as they lead to non-divergent terms. Finally, we note that the permutation of propagators inside such a pair leads to a symmetry factor of 1/2 for each pair. The factor of 1/2 introduced in the definition of $\mathcal{V}$ and Γ takes care of this.

The solution of the Bethe-Salpeter equation is given by

$$\mathcal{V} = (1 + \Gamma \diamond \mathcal{G}_0)^{-1} \diamond \Gamma \quad (2.41)$$

where the inverse is understood for the $\diamond$ product. The eigenvectors ψ of the operator $\Gamma \diamond \mathcal{G}_0$ are given by

$$\Gamma \diamond \mathcal{G}_0 \diamond \psi = \lambda \psi \quad (2.42)$$

The Cooper susceptibility $\mathcal{V}$ becomes divergent for $\lambda = -1$, marking the onset of superconductivity. The onset of superconductivity therefore corresponds to the solution of the following equation:

$$\frac{1}{\beta} \sum_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'} \Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}, \omega, \alpha, \sigma, \sigma'} (i\omega - \xi_{\mathbf{k}, \alpha})^{-1} (-i\omega - \xi_{-\mathbf{k}, \alpha})^{-1} \psi_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'} = -\psi_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1} \quad (2.43)$$

2.5.1 Frequency Dependence

One now needs to calculate Γ , which is the step where physical insight about the mechanism driving superconductivity is needed. We first treat the dependence of Γ on the Matsubara frequencies. For conventional superconductors, the effective interaction between electrons due to electron-phonon coupling is attractive at low frequencies and repulsive at high frequencies. Low and high frequencies are to be understood compared to the typical phonon frequency, the Debye frequency ω_D . An approximation for Γ that was shown to capture the right qualitative behaviour is then given by [14]:

$$\Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} = \begin{cases} \Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2}^{\text{Phon.}} & \text{if } |\omega_1|, |\omega_2| < \omega_D \\ 0 & \text{otherwise} \end{cases} \quad (2.44)$$

where $\Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2}^{\text{Phon.}}$ has a dominant short-range attractive component leading to the celebrated s -wave order parameter in conventional superconductors.

For a purely electronic mechanism, a natural cutoff would be of the order of the bare bandwidth $\omega_c \sim W \sim v_F k_F$. Actually, in a spin-fluctuation type scenario where the renormalized interaction is calculated from the random phase approximation, this cutoff is largely reduced if the Fermi liquid is close to a magnetic instability. Due to the proximity to this phase transition, the spin fluctuations exhibit a “critical slowing down” [17], whereby their velocity is reduced from the Fermi velocity: $v' \sim v_F(1 - \rho U)/\rho U$, where ρ is the density of states at the Fermi level. According to the Stoner criterion, the magnetic transition appears at $\rho U = 1$. Close to the transition, one has $\rho U = 1 - \eta$ with $\eta \ll 1$ and the cutoff is therefore strongly reduced: $\omega'_c \sim v' k_F \sim \eta W$. From the above discussion, it is clear that, in the limit $U/t \rightarrow 0$ treated in this thesis, the cutoff will be given by the bare bandwidth since $\rho U \rightarrow 0$.

Neglecting the frequency dependence of Γ apart from the presence of a cutoff, we will therefore take

$$\Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2} = \begin{cases} \Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2} & \text{if } |\omega_1|, |\omega_2| < \omega_c \\ 0 & \text{otherwise} \end{cases} \quad (2.45)$$

where, crucially, $\Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2}$ is repulsive at short distance but attractive at large distance, leading to unconventional order parameters. $\Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \alpha_2, \sigma_2, \sigma'_2}$ will be calculated perturbatively in the following.

A solution is now found by posing

$$\psi_{\mathbf{k}, \omega, \alpha, \sigma, \sigma'} = \begin{cases} \Delta_{\mathbf{k}, \alpha, \sigma, \sigma'} & \text{if } |\omega| < \omega_c \\ 0 & \text{otherwise} \end{cases} \quad (2.46)$$

and by rewriting Eq. 2.43 as

$$\frac{1}{\beta} \sum_{\mathbf{k}, \alpha, \sigma, \sigma'} \Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}, \alpha, \sigma, \sigma'} \Delta_{\mathbf{k}, \alpha, \sigma, \sigma'} \sum_{|\omega| < \omega_c} (i\omega - \xi_{\mathbf{k}, \alpha})^{-1} (-i\omega - \xi_{-\mathbf{k}, \alpha})^{-1} = -\Delta_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1}. \quad (2.47)$$

As usual, the frequency sum can be performed by substituting $i\omega$ by a complex variable z and using Cauchy's theorem:

$$\frac{1}{\beta} \sum_{|\omega| < \omega_c} g(i\omega) = \sum_j \text{Res}_{z=z_j} [g(z)] n_F(z_j) - \oint_{|z|=\omega_c} \frac{dz}{2\pi i} n_F(z) g(z) \quad (2.48)$$

where j indexes the poles of $g(z)$ enclosed by the contour defined by $|z| = \omega_c$ and where $n_F(z) = (e^{\beta z} + 1)^{-1}$. We want to apply this formula for $g(z) = (z - \xi_{\mathbf{k}, \alpha})^{-1} (-z - \xi_{-\mathbf{k}, \alpha})^{-1}$. For a given value of $\mathbf{k}$, the two poles in the complex plane are situated at $z = \pm \xi_{\mathbf{k}, \alpha}$. There are therefore two possibilities: either $\xi_{\mathbf{k}, \alpha} < \omega_c$ and the contour encloses these poles, or $\xi_{\mathbf{k}, \alpha} > \omega_c$ and it does not. Since the superconducting critical temperature T_c will emerge as a new energy scale exponentially smaller than the cutoff, one can assume $\beta\omega_c \gg 1$ and therefore neglect the second term in the right hand side of Eq. 2.48, leading to

$$\frac{1}{\beta} \sum_{|\omega| < \omega_c} (i\omega - \xi_{\mathbf{k}, \alpha})^{-1} (-i\omega - \xi_{-\mathbf{k}, \alpha})^{-1} \simeq \begin{cases} \frac{\tanh(\frac{1}{2}\beta\xi_{\mathbf{k}, \alpha})}{2\xi_{\mathbf{k}, \alpha}} & \text{if } |\xi_{\mathbf{k}, \alpha}| < \omega_c \\ 0 & \text{otherwise} \end{cases} \quad (2.49)$$

Going back to Eq. 2.47, the onset of superconductivity is controlled by the following equation:

$$\sum_{\alpha, \sigma, \sigma'} \sum'_{\mathbf{k}} \Gamma_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}, \alpha, \sigma, \sigma'} \Delta_{\mathbf{k}, \alpha, \sigma, \sigma'} \frac{\tanh(\frac{1}{2}\beta\xi_{\mathbf{k}, \alpha})}{2\xi_{\mathbf{k}, \alpha}} = -\Delta_{\mathbf{k}_1, \alpha_1, \sigma_1, \sigma'_1}. \quad (2.50)$$

where $\sum'_{\mathbf{k}}$ is a sum over all momenta such that $|\xi_{\mathbf{k}, \alpha}| < \omega_c$. This is the famous linearised gap equation [18], which can also be obtained by imposing self-consistency in a mean-field treatment of superconductivity, as explained in the following.

2.5.2 Solution of the Linearised Gap Equation

In order to solve the last equation, it is advantageous to rewrite the sum over momenta by a sum over $(\xi, \hat{\mathbf{k}})$, where $\hat{\mathbf{k}}$ lies on the iso-surface defined by $\xi_{\hat{\mathbf{k}},\alpha} = \xi$:

$$\sum_{\alpha} \sum_{\mathbf{k}} \dots = \sum_{\alpha} \int_{-\omega_c}^{\omega_c} d\xi \rho_{\xi,\alpha} \int_{S_{\xi,\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\xi,\alpha}|} \frac{\bar{v}_{\xi,\alpha}}{v_{\xi,\hat{\mathbf{k}},\alpha}} \dots \quad (2.51)$$

where $\rho_{\xi,\alpha} = \int_{S_{\xi,\alpha}} \frac{d\hat{\mathbf{k}}}{(2\pi)^D} \frac{1}{v_{\xi,\hat{\mathbf{k}},\alpha}}$ is the density of states of band α at energy ξ , $S_{\xi,\alpha}$ is the Fermi surface of band α at energy ξ , $|S_{\xi,\alpha}|$ is the area of this Fermi surface, $v_{\xi,\hat{\mathbf{k}},\alpha}$ is the group velocity of band α at energy ξ and momentum $\hat{\mathbf{k}}$, and $\bar{v}_{\xi,\alpha} = \left(\int_{S_{\xi,\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\xi,\alpha}|} \frac{1}{v_{\xi,\hat{\mathbf{k}},\alpha}} \right)^{-1}$ its average.

The gap equation can be rewritten as

$$\int_{-\omega_c}^{\omega_c} d\xi f(\xi) \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{2\xi} = -\Delta_{(\xi_1, \hat{\mathbf{k}}_1), \alpha_1, \sigma_1, \sigma'_1} \quad (2.52)$$

with

$$f(\xi) \equiv \sum_{\alpha} \rho_{\xi,\alpha} \int_{S_{\xi,\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\xi,\alpha}|} \frac{\bar{v}_{\xi,\alpha}}{v_{\xi,\hat{\mathbf{k}},\alpha}} \sum_{\sigma, \sigma'} \Gamma_{(\xi_1, \hat{\mathbf{k}}_1), \alpha_1, \sigma_1, \sigma'_1; (\xi, \hat{\mathbf{k}}), \alpha, \sigma, \sigma'} \Delta_{(\xi, \hat{\mathbf{k}}), \alpha, \sigma, \sigma'} \quad (2.53)$$

Due to the $\tanh\left(\frac{\beta\xi}{2}\right)/2\xi$ factor, the sum is dominated by behaviour at small ξ , and we can use the following Taylor expansion:

$$f(\xi) = f(0) + f'(0)\xi + \frac{1}{2}f''(0)\xi^2 + \dots \quad (2.54)$$

This leads to

$$\int_{-\omega_c}^{\omega_c} d\xi f(\xi) \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{2\xi} = f(0) \log\left(\frac{2e^{\gamma}\beta\omega_c}{\pi}\right) + \dots \quad (2.55)$$

where $\dots$ stands for terms that are regular in the $T \rightarrow 0$ limit. These terms would lead to multiplicative factors of order one for T_c , which we will neglect.

Finally, the gap equation becomes

$$\sum_{\alpha} \rho_{\alpha} \int_{S_{\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\alpha}|} \frac{\bar{v}_{\alpha}}{v_{\hat{\mathbf{k}},\alpha}} \sum_{\sigma, \sigma'} \Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}, \alpha, \sigma, \sigma'} \Delta_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'} = -\log\left(\frac{2e^{\gamma}\beta\omega_c}{\pi}\right)^{-1} \Delta_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1} \quad (2.56)$$

where all quantities are evaluated at the Fermi level.

It is now advantageous to introduce the dimensionless pairing matrix g and its eigenmodes defined by

$$\sum_{\alpha} \sum_{\sigma, \sigma'} \int_{S_{\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\alpha}|} g_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}, \alpha, \sigma, \sigma'} \varphi_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'} = \lambda \varphi_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1} \quad (2.57)$$

where

$$g_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \equiv \sqrt{\rho_{\alpha_1} \frac{\bar{v}_{\alpha_1}}{v_{\hat{\mathbf{k}}_1, \alpha_1}}} \Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \sqrt{\rho_{\alpha_2} \frac{\bar{v}_{\alpha_2}}{v_{\hat{\mathbf{k}}_2, \alpha_2}}}. \quad (2.58)$$

Since Γ is non-singular in the limit $T \rightarrow 0$ and we expect $T_c \ll W$, we neglect the temperature dependence of Γ and we will compute it at $T = 0$ in the next section.

For each $\lambda < 0$, we have a solution of the linearised gap equation given by

$$T_c = \mathcal{W} \exp\left(\frac{1}{\lambda}\right) \quad (2.59)$$

$$\Delta_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'} \propto \tilde{\varphi}_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'} \equiv \sqrt{\frac{\rho_{\alpha} \bar{v}_{\alpha}}{v_{\hat{\mathbf{k}}, \alpha}}}^{-1} \varphi_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'}$$

where $\mathcal{W} = \frac{2e^{\gamma}\omega_c}{\pi} \simeq 1.13 \omega_c$ is of the order of the bandwidth. By solving the eigenproblem of Eq. 2.57, we thus obtain T_c from the eigenvalue and the order parameter Δ from the eigenvector. The eigenmode with the most negative eigenvalue corresponds to the order parameter with the highest T_c . After discretization of the Fermi surfaces, g becomes a hermitian matrix that is readily diagonalized numerically.

Note that the eigenvectors of g are orthonormal:

$$\sum_{\alpha} \sum_{\sigma, \sigma'} \int_{S_{\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\alpha}|} \left(\varphi_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'}^{(i)} \right)^* \varphi_{\hat{\mathbf{k}}, \alpha, \sigma, \sigma'}^{(j)} = \delta_{i,j} \quad (2.60)$$

where i and j are eigenvector indices.

2.6 Calculation of the Effective Interaction

What is now left to do is to compute Γ at leading order in U/t for the interaction given in Eq. 2.17 by using the Feynman rules given in Sect. 2.4.1. As a reminder, $\Gamma_{\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1, \sigma'_1; \mathbf{k}_2, \omega_2, \alpha_2, \sigma_2, \sigma'_2}$ is defined as the sum of all connected, irreducible diagrams with two outgoing external legs $(\mathbf{k}_2, \omega_2, \alpha_2, \sigma_2$ and $-\mathbf{k}_2, -\omega_2, \alpha_2, \sigma'_2)$ and two incoming external legs $(\mathbf{k}_1, \omega_1, \alpha_1, \sigma_1$ and $-\mathbf{k}_1, -\omega_1, \alpha_1, \sigma'_1)$, where the external propagators and Delta functions are stripped off, and where an overall factor

Fig. 2.4 Only diagram at order U

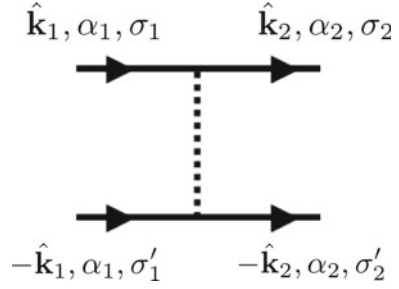


Fig. 2.5 First diagram at order U^2 . The external legs have $\omega = 0$

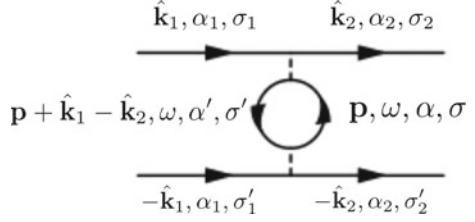
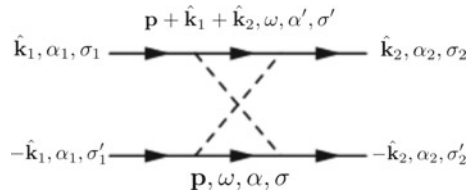


Fig. 2.6 Second diagram at order U^2 . The external legs have $\omega = 0$



of $\frac{1}{2}$ is added (see Fig. 2.2). Given the results of last section, we will only need the zero frequency components of the effective interaction: $\Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2}^{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2} \equiv \Gamma_{\hat{\mathbf{k}}_1, \omega_1=0, \alpha_1, \sigma_1; \hat{\mathbf{k}}_2, \omega_2=0, \alpha_2, \sigma_2}$. The external propagators of our diagrams will therefore have $\omega = 0$.

At order U , there is only one diagram, shown in Fig. 2.4. Its contribution to Γ is

$$\Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2}^{(1)} = \frac{1}{2} V_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1; -\hat{\mathbf{k}}_1, \alpha_1, \sigma'_1; -\hat{\mathbf{k}}_2, \alpha_2, \sigma'_2; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2}. \quad (2.61)$$

As a reminder, in the case of a single-orbital, spin $SU(2)$ -symmetric Hubbard model, the interaction is given by

$$V_{s_1, s'_1; s'_2, s_2}^{\text{Hub.}} = U \delta_{s_1, -s'_1} \delta_{s_2, -s'_2} (\delta_{s'_1, s'_2} - \delta_{s'_1, s_2}). \quad (2.62)$$

This would lead to

$$\Gamma_{\hat{\mathbf{k}}_1, s_1, s'_1; \hat{\mathbf{k}}_2, s_2, s'_2}^{(1), \text{Hub.}} = \frac{1}{2} U \delta_{s_1, -s'_1} \delta_{s_2, -s'_2} (\delta_{s'_1, s'_2} - \delta_{s'_1, s_2}). \quad (2.63)$$

At order U^2 , there are two diagrams, given in Figs. 2.5 and 2.6. Their contribution can be expressed in terms of the following function:

$$F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \equiv - \sum_{\alpha, \alpha', \sigma, \sigma'} \sum_{\mathbf{p}} \frac{1}{\beta} \sum_{\omega} (i\omega - \xi_{\mathbf{p}, \alpha})^{-1} (i\omega - \xi_{\mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha'})^{-1} \\ V_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \mathbf{p}, \alpha, \sigma; \mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha', \sigma'; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2} V_{-\hat{\mathbf{k}}_1, \alpha_1, \sigma'_1; \mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha', \sigma'; \mathbf{p}, \alpha, \sigma; -\hat{\mathbf{k}}_2, \alpha_2, \sigma'_2}. \quad (2.64)$$

In terms of this function, we have

$$\Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2}^{(2)} = \frac{1}{2} \left(-F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} + F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; -\hat{\mathbf{k}}_2, \alpha_2, \sigma'_2, \sigma_2} \right) \quad (2.65)$$

where the first term corresponds to the first diagram, and the second term corresponds to the second diagram. The minus sign comes from the fermionic loop in the first diagram. We can now evaluate the Matsubara sum, leading to

$$F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} = - \sum_{\alpha, \alpha', \sigma, \sigma'} \sum_{\mathbf{p}} \frac{n(\xi_{\mathbf{p}, \alpha}) - n(\xi_{\mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha'})}{\xi_{\mathbf{p}, \alpha} - \xi_{\mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha'}} \quad (2.66) \\ V_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \mathbf{p}, \alpha, \sigma; \mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha', \sigma'; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2} V_{-\hat{\mathbf{k}}_1, \alpha_1, \sigma'_1; \mathbf{p} + \hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2, \alpha', \sigma'; \mathbf{p}, \alpha, \sigma; -\hat{\mathbf{k}}_2, \alpha_2, \sigma'_2}.$$

This function can be computed numerically by using the tetrahedron method [19]. Within the approximations made above, one can neglect the temperature dependence of this function and compute it at $T = 0$.

Note that in the single-orbital case, this function would simply be given by

$$F_{\hat{\mathbf{k}}_1, s_1, s'_1; \hat{\mathbf{k}}_2, s_2, s'_2}^{\text{Hub.}} = U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2) (\delta_{s_1, s'_1} \delta_{s_2, s'_2} \delta_{s_1, s_2} + \delta_{s_1, -s'_1} \delta_{s_2, -s'_2} \delta_{s_1, -s_2}) \quad (2.67)$$

where $\chi^{\text{ph}}(\mathbf{q})$ is the Lindhard susceptibility, defined by

$$\chi^{\text{ph}}(\mathbf{q}) = - \sum_{\mathbf{p}} \frac{n(\xi_{\mathbf{p}}) - n(\xi_{\mathbf{p} + \mathbf{q}})}{\xi_{\mathbf{p}} - \xi_{\mathbf{p} + \mathbf{q}}}. \quad (2.68)$$

2.6.1 Pseudo-spin Dependence

When looking for the eigenmodes $\varphi_{\mathbf{k}, \alpha, \sigma, \sigma'}$ of the effective interaction, it is advantageous to go to the aforementioned pseudo-spin basis, since Γ has a block-diagonal structure in that basis. The pseudo-spin transformation separates the pseudo-spin degrees of freedom in a singlet φ_{d_0} and a triplet $\varphi_{\vec{d}}$:

$$\begin{pmatrix} \varphi_{++} & \varphi_{+-} \\ \varphi_{-+} & \varphi_{--} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\varphi_{d_x} + i\varphi_{d_y} & \varphi_{d_z} + \varphi_{d_0} \\ \varphi_{d_z} - \varphi_{d_0} & \varphi_{d_x} + i\varphi_{d_y} \end{pmatrix}, \quad (2.69)$$

where we have left the indices $\mathbf{k}, \alpha$ implicit. Using this unitary transformation on $\Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2}$, we obtain $\Gamma_{\hat{\mathbf{k}}_1, \alpha_1, d_{\mu,1}; \hat{\mathbf{k}}_2, \alpha_2, d_{\mu,1}}$ with $\mu = 0, x, y, z$.

In the following, we will use the notation $\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2}$ for the matrix

$$(\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \equiv \Gamma_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \quad (2.70)$$

and $\Gamma_{d_{\mu,1}; d_{\mu,2}}$ for the matrix

$$(\Gamma_{d_{\mu,1}; d_{\mu,2}})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \equiv \Gamma_{\hat{\mathbf{k}}_1, \alpha_1, d_{\mu,1}; \hat{\mathbf{k}}_2, \alpha_2, d_{\mu,2}}. \quad (2.71)$$

Using inversion symmetry, we find $\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2} = \Gamma_{\sigma'_1, \sigma_1; \sigma'_2, \sigma_2}$. Using this last relation, we find $\Gamma_{d_0; \vec{d}} = 0$, which means that the pseudo-spin singlet and triplet channels are decoupled.

Furthermore, Γ is invariant under the double group symmetry operations discussed in Sect. 2.3.1:

$$\begin{aligned} \mathcal{R}(\Gamma_{d_0; d_0})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \mathcal{R}^{-1} &\equiv (\Gamma_{d_0; d_0})_{\mathcal{R}\hat{\mathbf{k}}_1, \alpha_1; \mathcal{R}\hat{\mathbf{k}}_2, \alpha_2} = (\Gamma_{d_0; d_0})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \\ \mathcal{R}(\Gamma_{\vec{d}; \vec{d}})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \mathcal{R}^{-1} &\equiv (\Gamma_{\mathcal{R}\vec{d}; \mathcal{R}\vec{d}})_{\mathcal{R}\hat{\mathbf{k}}_1, \alpha_1; \mathcal{R}\hat{\mathbf{k}}_2, \alpha_2} = (\Gamma_{\vec{d}; \vec{d}})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2}. \end{aligned} \quad (2.72)$$

This means that its eigenvectors can be classified according to the irreducible representations of the point group.

As explained in Sect. 3.2.2, the interaction considered for the case of Sr_2RuO_4 actually conserves total pseudo-spin modulo 4 thanks to a $z \rightarrow -z$ mirror symmetry. In that case, $\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2}$ is non-zero only when $\frac{1}{2}(\sigma_1 + \sigma'_1) = \frac{1}{2}(\sigma_2 + \sigma'_2) \pmod{2}$ (which means that $\Gamma_{+1, -1; +1, +1} = 0$ for example) and the d_z and the d_x, d_y sectors are therefore not coupled. In matrix form, one can write $\Gamma_{d_{\mu,1}; d_{\mu,2}}$ as

$$\begin{pmatrix} \Gamma_{d_0, d_0} & 0 & 0 & 0 \\ 0 & \Gamma_{d_z, d_z} & 0 & 0 \\ 0 & 0 & \Gamma_{d_x, d_x} & \Gamma_{d_x, d_y} \\ 0 & 0 & \Gamma_{d_y, d_x} & \Gamma_{d_y, d_y} \end{pmatrix} \quad (2.73)$$

in the basis $[d_0, d_z, d_x, d_y]$. The matrix elements are given by

$$\begin{aligned} \Gamma_{d_0, d_0} &= \Gamma_{+-; +-} - \Gamma_{+-; -+} \\ \Gamma_{d_z, d_z} &= \Gamma_{+-; +-} + \Gamma_{+-; -+} \\ \Gamma_{d_x, d_x} &= \frac{1}{2}(\Gamma_{++; ++} - \Gamma_{++; --} - \Gamma_{--; ++} + \Gamma_{--; --}) \\ \Gamma_{d_x, d_y} &= i\frac{1}{2}(-\Gamma_{++; ++} - \Gamma_{++; --} + \Gamma_{--; ++} + \Gamma_{--; --}) \\ \Gamma_{d_y, d_x} &= -i\frac{1}{2}(-\Gamma_{++; ++} + \Gamma_{++; --} - \Gamma_{--; ++} + \Gamma_{--; --}) \\ \Gamma_{d_y, d_y} &= \frac{1}{2}(\Gamma_{++; ++} + \Gamma_{++; --} + \Gamma_{--; ++} + \Gamma_{--; --}). \end{aligned} \quad (2.74)$$

We can now inject the formulas found for $\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2}$ in the last section. It is advantageous to define the following matrices

$$(F_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2}^{\pm})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} = -\frac{1}{2} \left(F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; \hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \pm F_{\hat{\mathbf{k}}_1, \alpha_1, \sigma_1, \sigma'_1; -\hat{\mathbf{k}}_2, \alpha_2, \sigma_2, \sigma'_2} \right). \quad (2.75)$$

The operator F^+ (F^-) is non-zero only in the even (odd) parity subspace, defined by $\varphi_{\hat{\mathbf{k}}, \alpha} = \varphi_{-\hat{\mathbf{k}}, \alpha}$ ($\varphi_{\hat{\mathbf{k}}, \alpha} = -\varphi_{-\hat{\mathbf{k}}, \alpha}$).

2.6.1.1 Pseudo-spin Triplet

Using inversion symmetry and the fact that we have an on-site interaction, it is easy to see that $\Gamma_{\sigma_1, \sigma'_1; \sigma_2, \sigma'_2}^{(1)} = -\Gamma_{\sigma_1, \sigma'_1; \sigma'_2, \sigma_2}^{(1)} = -\Gamma_{\sigma'_1, \sigma_1; \sigma_2, \sigma'_2}^{(1)}$. The order U term is therefore zero in the triplet channel.

As mentioned previously, there are two decoupled sectors, corresponding to two different orientations of $\vec{d}$: out-of-plane (d_z) and in-plane (d_x, d_y). Since the order U term is zero, we go directly to the order U^2 term. In the d_z case, the effective interaction is given by

$$\Gamma_{d_z, d_z}^{(2)} = F_{+, -, +, -}^- + F_{+, -, -, +}^-. \quad (2.76)$$

In the in-plane case, the effective interaction is given by

$$\begin{aligned} \Gamma_{d_x, d_x}^{(2)} &= \frac{1}{2} (F_{+, +, +, +}^- - F_{+, +, -, -}^- - F_{-, -, +, +}^- + F_{-, -, -, -}^-) \\ \Gamma_{d_x, d_y}^{(2)} &= i \frac{1}{2} (-F_{+, +, +, +}^- - F_{+, +, -, -}^- + F_{-, -, +, +}^- + F_{-, -, -, -}^-) \\ \Gamma_{d_y, d_x}^{(2)} &= -i \frac{1}{2} (-F_{+, +, +, +}^- + F_{+, +, -, -}^- - F_{-, -, +, +}^- + F_{-, -, -, -}^-) \\ \Gamma_{d_y, d_y}^{(2)} &= \frac{1}{2} (F_{+, +, +, +}^- + F_{+, +, -, -}^- + F_{-, -, +, +}^- + F_{-, -, -, -}^-). \end{aligned} \quad (2.77)$$

In the single-orbital Hubbard case, this would lead to

$$(\Gamma_{d_z, d_z}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} = \frac{1}{2} \left(U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2) - U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2) \right) \quad (2.78)$$

and

$$\begin{aligned} (\Gamma_{d_x, d_x}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} &= \frac{1}{2} (U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2) - U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)) \\ (\Gamma_{d_x, d_y}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} &= 0 \\ (\Gamma_{d_y, d_x}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} &= 0 \\ (\Gamma_{d_y, d_y}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} &= \frac{1}{2} (U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2) - U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)). \end{aligned} \quad (2.79)$$

In the single-orbital Hubbard model case, Γ is isotropic in $\vec{d}$, since, without spin-orbit coupling, the system is $SU(2)$ invariant. This is not the case in general since the in-plane and out-of-plane sectors of Γ are in general different. In the next Chapter, we will show how the difference between the in-plane and out-of-plane sectors due to spin-orbit coupling favours certain order parameters in Sr_2RuO_4 .

2.6.1.2 Pseudo-spin Singlet

In the singlet channel, the order U term is non-zero:

$$(\Gamma_{d_0, d_0}^{(1)})_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} = V_{\hat{\mathbf{k}}_1, \alpha_1, +, -; -\hat{\mathbf{k}}_2, \alpha_2, -, +}. \quad (2.80)$$

In the single-orbital Hubbard case, one would have

$$(\Gamma_{d_0, d_0}^{(1), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} = U. \quad (2.81)$$

If $\Gamma_{d_0, d_0}^{(1)}$ has at least one negative eigenvalue, the most negative one gives the leading instability in the pseudo-spin singlet channel, and there is no need to look at order U^2 . This is what would happen for the attractive single-orbital Hubbard model, i.e. for $U < 0$.

Instead, in the case of a repulsive bare interaction, relevant to electrons in a solid, the eigenvalues of $\Gamma_{d_0, d_0}^{(1)}$ will be either positive or zero, and there will therefore be no divergence at order U . Nevertheless, a negative eigenvalue could appear at order U^2 in the subspace $\mathcal{S}$ defined by the zero eigenvalues of $\Gamma_{d_0, d_0}^{(1)}$. One should therefore diagonalize $P_{\mathcal{S}} \Gamma_{d_0, d_0}^{(2)} P_{\mathcal{S}}$, where $P_{\mathcal{S}}$ is the projector onto $\mathcal{S}$ and where

$$\Gamma_{d_0, d_0}^{(2)} = F_{+, -, +, -}^+ - F_{+, -, -, +}^+. \quad (2.82)$$

In the single-orbital Hubbard case, the space $\mathcal{S}$ is easily defined: it is the space of all $\varphi_{\hat{\mathbf{k}}}$ such that $\sum_{\hat{\mathbf{k}}} \varphi_{\hat{\mathbf{k}}} = 0$. The uniform s -wave order parameter $\varphi_{\hat{\mathbf{k}}} = \varphi \forall \hat{\mathbf{k}}$ present in conventional superconductors is therefore disfavored because of the bare repulsion. On the other hand, all order parameters in non-trivial (i.e. non s -wave) irreducible representations of the point group¹ are contained in $\mathcal{S}$ since they satisfy $\sum_{\hat{\mathbf{k}}} \varphi_{\hat{\mathbf{k}}} = 0$ by symmetry. For example, on a square lattice, these non-trivial representations would be given by A_{2g} , B_{1g} and B_{2g} as shown in Table 5.3. In order to find the most favored of these order parameters, one should diagonalize $P_{\mathcal{S}} \Gamma_{d_0, d_0}^{(2)} P_{\mathcal{S}}$, with

$$(\Gamma_{d_0, d_0}^{(2), \text{Hub.}})_{\hat{\mathbf{k}}_1; \hat{\mathbf{k}}_2} = \frac{1}{2} \left(U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2) + U^2 \chi^{\text{ph}}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2) \right). \quad (2.83)$$

¹One should of course only consider even-parity representations in the singlet channel in order to satisfy the Pauli principle.

2.7 Generalized BCS Formalism

In the last sections, we have established the presence of a divergence of the susceptibility to Cooper pairing at a critical temperature T_c , corresponding to the most negative eigenvalue of the effective interaction in the Cooper channel. The momentum and band anisotropy of the order parameter was then shown to be given by the corresponding eigenvector. The motivation came from a system in which an infinitesimally small field couples directly to the order parameter. While this technique works well to study the superconducting instability coming from the Fermi liquid, it is not well suited to the study of the system below T_c .

Instead, in order to study the superconducting phase, it would be advantageous to use the Bardeen-Cooper-Schrieffer (BCS) formalism [2] generalized to anisotropic, spin-orbit coupled, multi-orbital systems. We start from a reduced BCS Hamiltonian of the following form:

$$H_{BCS} = H_K + \frac{1}{2} \sum_{\alpha_1, d_{\mu_1}} \sum_{\alpha_2, d_{\mu_2}} \sum'_{\mathbf{k}_1, \mathbf{k}_2} V_{\mathbf{k}_1, \alpha_1, d_{\mu_1}; \mathbf{k}_2, \alpha_2, d_{\mu_2}}^{BCS} \phi_{\mathbf{k}_1, \alpha_1, d_{\mu_1}}^\dagger \phi_{\mathbf{k}_2, \alpha_2, d_{\mu_2}} \quad (2.84)$$

where H_K is the single-particle part of the Hamiltonian defined in Eq. 2.17, ϕ was defined in Eq. 2.26 and $\sum'_{\mathbf{k}_1, \mathbf{k}_2}$ is a sum over momenta such that $|\xi_{\mathbf{k}_1, \alpha_1}|, |\xi_{\mathbf{k}_2, \alpha_2}| < \omega_c$. In the following, we will omit the ' on the sum symbols, but all sums over momenta should be taken with that energy cutoff. Using the effective interaction calculated in the previous sections, we take

$$V_{\mathbf{k}_1, \alpha_1, d_{\mu_1}; \mathbf{k}_2, \alpha_2, d_{\mu_2}}^{BCS} = \Gamma_{\mathbf{k}_1, \alpha_1, d_{\mu_1}; \mathbf{k}_2, \alpha_2, d_{\mu_2}}. \quad (2.85)$$

We now follow the standard mean-field treatment of this Hamiltonian, by assuming the following two operators acquire a non-zero expectation value

$$\begin{aligned} \Delta_{\mathbf{k}_1, \alpha_1, d_{\mu_1}} &= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_2, \alpha_2, d_{\mu_2}} V_{\mathbf{k}_1, \alpha_1, d_{\mu_1}; \mathbf{k}_2, \alpha_2, d_{\mu_2}}^{BCS} \langle \phi_{\mathbf{k}_2, \alpha_2, d_{\mu_2}} \rangle \\ \bar{\Delta}_{\mathbf{k}_2, \alpha_2, d_{\mu_2}} &= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_1, \alpha_1, d_{\mu_1}} \langle \phi_{\mathbf{k}_1, \alpha_1, d_{\mu_1}}^\dagger \rangle V_{\mathbf{k}_1, \alpha_1, d_{\mu_1}; \mathbf{k}_2, \alpha_2, d_{\mu_2}}^{BCS}. \end{aligned} \quad (2.86)$$

Using these formulas, and neglecting fluctuations, we obtain

$$H_{BCS} = H_K + \frac{1}{2} \sqrt{2} \sum_{\mathbf{k}, \alpha, d_\mu} (\Delta_{\mathbf{k}, \alpha, d_\mu} \phi_{\mathbf{k}, \alpha, d_\mu}^\dagger + \bar{\Delta}_{\mathbf{k}, \alpha, d_\mu} \phi_{\mathbf{k}, \alpha, d_\mu}) + \bar{\Delta} (V^{BCS})^{-1} \Delta \quad (2.87)$$

with

$$\bar{\Delta}(V^{BCS})^{-1}\Delta = \sum_{\mathbf{k}_1, \alpha_1, d_{\mu,1}} \sum_{\mathbf{k}_2, \alpha_2, d_{\mu,2}} \bar{\Delta}_{\mathbf{k}_1, \alpha_1, d_{\mu,1}} (V^{BCS})_{\mathbf{k}_1, \alpha_1, d_{\mu,1}; \mathbf{k}_2, \alpha_2, d_{\mu,2}}^{-1} \Delta_{\mathbf{k}_2, \alpha_2, d_{\mu,2}}. \quad (2.88)$$

This Hamiltonian is now quadratic and can be rewritten as

$$H_{BCS} = \frac{1}{2} \sum_{\mathbf{k}, \alpha} \psi_{\mathbf{k}, \alpha}^{\dagger} \mathcal{H}_{\mathbf{k}, \alpha} \psi_{\mathbf{k}, \alpha} + \text{Constant} \quad (2.89)$$

with $\psi_{\mathbf{k}, \alpha}^{\dagger} = [c_{\mathbf{k}, \alpha, +}^{\dagger}, c_{\mathbf{k}, \alpha, -}^{\dagger}, c_{-\mathbf{k}, \alpha, +}, c_{-\mathbf{k}, \alpha, -}]$ and

$$\mathcal{H}_{\mathbf{k}, \alpha} = \begin{pmatrix} \xi_{\mathbf{k}, \alpha} & 0 & -\Delta_{\mathbf{k}, \alpha, d_x} + i\Delta_{\mathbf{k}, \alpha, d_y} & \Delta_{\mathbf{k}, \alpha, d_z} + \Delta_{\mathbf{k}, \alpha, d_0} \\ 0 & \xi_{\mathbf{k}, \alpha} & \Delta_{\mathbf{k}, \alpha, d_z} - \Delta_{\mathbf{k}, \alpha, d_0} & \Delta_{\mathbf{k}, \alpha, d_x} + i\Delta_{\mathbf{k}, \alpha, d_y} \\ -\bar{\Delta}_{\mathbf{k}, \alpha, d_x} - i\bar{\Delta}_{\mathbf{k}, \alpha, d_y} & \bar{\Delta}_{\mathbf{k}, \alpha, d_z} - \bar{\Delta}_{\mathbf{k}, \alpha, d_0} & -\xi_{\mathbf{k}, \alpha} & 0 \\ \bar{\Delta}_{\mathbf{k}, \alpha, d_z} + \bar{\Delta}_{\mathbf{k}, \alpha, d_0} & \bar{\Delta}_{\mathbf{k}, \alpha, d_x} - i\bar{\Delta}_{\mathbf{k}, \alpha, d_y} & 0 & -\xi_{\mathbf{k}, \alpha} \end{pmatrix}. \quad (2.90)$$

Note that we used inversion symmetry to write $\xi_{\mathbf{k}, \alpha} = \xi_{-\mathbf{k}, \alpha}$.

In the previous sections, we diagonalized Γ (more precisely, the pairing matrix g), and we showed that each mode provides a distinct solution of the linearized gap equation with a different value of T_c . These modes are classified according to the irreducible representations of the point group of the lattice. While this works for identifying the mode with the highest T_c , these modes actually become coupled in the superconducting phase when one goes beyond the linearized version of the self-consistency equation, or equivalently, when one includes quartic terms in the Ginzburg-Landau formalism. In general, one should therefore solve H_{BCS} for all temperatures, and the functional form of the gap can generically have a temperature dependence.

Instead, we make the usual approximation that the order parameter functional form is temperature independent, and that only its overall magnitude depends on T [20]:

$$\Delta_{\mathbf{k}, \alpha, d_{\mu}}(T) = \Delta(T) \tilde{\varphi}_{\mathbf{k}, \alpha, d_{\mu}} \quad (2.91)$$

where $\tilde{\varphi}_{\mathbf{k}, \alpha, d_{\mu}}$ is the mode found in Sect. 2.5, normalized so that

$$\max_{\mathbf{k}, \alpha} \sum_{\mu} |\tilde{\varphi}_{\mathbf{k}, \alpha, d_{\mu}}|^2 = 1 \quad (2.92)$$

and where $\Delta(T)$ sets the energy scale of the gap.

2.7.1 Singlet

Let us now discuss different cases. As explained in the previous section, in an inversion-symmetric problem, one can always distinguish between pseudo-spin singlet and triplet. In the singlet case, the only non-zero component of the gap is $\Delta_{\mathbf{k},\alpha,d_0}$. For notational convenience, we define $\Delta_{\mathbf{k},\alpha,d_0} \equiv \Delta_{\mathbf{k},\alpha}$ and the Hamiltonian becomes

$$\mathcal{H}_{\mathbf{k},\alpha} = \begin{pmatrix} \xi_{\mathbf{k},\alpha} & 0 & 0 & \Delta_{\mathbf{k},\alpha} \\ 0 & \xi_{\mathbf{k},\alpha} & -\Delta_{\mathbf{k},\alpha} & 0 \\ 0 & -\overline{\Delta_{\mathbf{k},\alpha}} & -\xi_{\mathbf{k},\alpha} & 0 \\ \overline{\Delta_{\mathbf{k},\alpha}} & 0 & 0 & -\xi_{\mathbf{k},\alpha} \end{pmatrix}. \quad (2.93)$$

Since this matrix can be split into two decoupled blocks, the Hamiltonian can be split into two terms. Using $\Delta_{\mathbf{k},\alpha} = \Delta_{-\mathbf{k},\alpha}$ coming from fermionic statistics, it is easy to see that these two terms are the same, and we therefore only need to diagonalize one of the blocks. Since the Hamiltonian is block diagonal in band space, we can diagonalize each band separately and omit the band index for now. We can now diagonalize the Hamiltonian using a Bogolyubov transformation:

$$\begin{aligned} c_{\mathbf{k},+}^\dagger &= v'_\mathbf{k} a_\mathbf{k}^\dagger + v_\mathbf{k}^* b_\mathbf{k} \\ c_{-\mathbf{k},-}^\dagger &= v'_\mathbf{k} b_\mathbf{k}^\dagger - v_\mathbf{k}^* a_\mathbf{k} \end{aligned} \quad (2.94)$$

with

$$\begin{aligned} v'_\mathbf{k} &= i e^{-i\Theta_\mathbf{k}/2} \cos(\theta_\mathbf{k}) \\ v_\mathbf{k} &= -i e^{i\Theta_\mathbf{k}/2} \sin(\theta_\mathbf{k}) \\ \cot(2\theta_\mathbf{k}) &= \frac{\xi_\mathbf{k}}{|\Delta_\mathbf{k}|} \end{aligned} \quad (2.95)$$

where we have parametrized the gap as $\Delta_\mathbf{k} = |\Delta_\mathbf{k}| e^{i\Theta_\mathbf{k}}$ and where $|v'_\mathbf{k}|^2 + |v_\mathbf{k}|^2 = 1$ in order to preserve anticommutation relations. We also give the inverse transformation for later convenience:

$$\begin{aligned} a_\mathbf{k}^\dagger &= (v'_\mathbf{k})^* c_{\mathbf{k},+}^\dagger - v_\mathbf{k}^* c_{-\mathbf{k},-} \\ b_\mathbf{k}^\dagger &= (v'_\mathbf{k})^* c_{-\mathbf{k},-}^\dagger + v_\mathbf{k}^* c_{\mathbf{k},+} \end{aligned} \quad (2.96)$$

The Hamiltonian now reads

$$H_{BCS} = \sum_{\mathbf{k},\alpha} E_{\mathbf{k},\alpha} (a_{\mathbf{k},\alpha}^\dagger a_{\mathbf{k},\alpha} + b_{\mathbf{k},\alpha}^\dagger b_{\mathbf{k},\alpha}) + \sum_{\mathbf{k},\alpha} (\xi_{\mathbf{k},\alpha} - E_{\mathbf{k},\alpha}) + \overline{\Delta} (V^{BCS})^{-1} \Delta \quad (2.97)$$

where $E_{\mathbf{k},\alpha} = \sqrt{\xi_{\mathbf{k},\alpha}^2 + |\Delta_{\mathbf{k},\alpha}|^2}$.

The gap equation is now obtained by imposing self-consistency:

$$\begin{aligned}
\Delta_{\mathbf{k}_1, \alpha_1} &= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_2, \alpha_2} V_{\mathbf{k}_1, \alpha_1; \mathbf{k}_2, \alpha_2}^{BCS} \langle \phi_{\mathbf{k}_2, \alpha_2} \rangle \\
&= \sum_{\mathbf{k}_2, \alpha_2} V_{\mathbf{k}_1, \alpha_1; \mathbf{k}_2, \alpha_2}^{BCS} (v'_{\mathbf{k}_2, \alpha_2})^* v_{\mathbf{k}_2, \alpha_2} \left(1 - \langle a_{\mathbf{k}_2, \alpha_2}^\dagger a_{\mathbf{k}_2, \alpha_2} \rangle - \langle b_{\mathbf{k}_2, \alpha_2}^\dagger b_{\mathbf{k}_2, \alpha_2} \rangle \right) \\
&= - \sum_{\mathbf{k}_2, \alpha_2} V_{\mathbf{k}_1, \alpha_1; \mathbf{k}_2, \alpha_2}^{BCS} \Delta_{\mathbf{k}_2, \alpha_2} \frac{\tanh(E_{\mathbf{k}_2, \alpha_2}/2T)}{2E_{\mathbf{k}_2, \alpha_2}}
\end{aligned} \tag{2.98}$$

where the d_0 index is implicit.

At $T = 0$, the gap equation becomes

$$\Delta_{\mathbf{k}_1, \alpha_1} = - \sum_{\mathbf{k}_2, \alpha_2} V_{\mathbf{k}_1, \alpha_1; \mathbf{k}_2, \alpha_2}^{BCS} \Delta_{\mathbf{k}_2, \alpha_2} \frac{1}{2E_{\mathbf{k}_2, \alpha_2}}. \tag{2.99}$$

The sum over momenta is again dominated by the Fermi surface contribution due to the $1/E_{\mathbf{k}, \alpha}$ factor. Using the same Taylor expansion used in Sect. 2.5.2, one finds

$$\varphi_{\hat{\mathbf{k}}_1, \alpha_1} = - \sum_{\alpha_2} \int_{S_{\alpha_2}} \frac{d\hat{\mathbf{k}}_2}{|S_{\alpha_2}|} g_{\hat{\mathbf{k}}_1, \alpha_1; \hat{\mathbf{k}}_2, \alpha_2} \varphi_{\hat{\mathbf{k}}_2, \alpha_2} \int_{-\omega_c}^{\omega_c} d\xi \frac{1}{2E_{\mathbf{k}_2, \alpha_2}}. \tag{2.100}$$

After performing the integral over ξ , the equation becomes

$$\varphi_{\hat{\mathbf{k}}_1, \alpha_1} = - \sum_{\alpha_2} \int_{S_{\alpha_2}} \frac{d\hat{\mathbf{k}}_2}{|S_{\alpha_2}|} g_{\hat{\mathbf{k}}_1, \alpha_1, d_0; \hat{\mathbf{k}}_2, \alpha_2, d_0} \varphi_{\hat{\mathbf{k}}_2, \alpha_2} \log \left(\frac{2\omega_c}{\Delta(0) |\tilde{\varphi}_{\hat{\mathbf{k}}_2, \alpha_2}|} \right) \tag{2.101}$$

where φ and $\tilde{\varphi}$ were defined in Sect. 2.5.2. We choose the normalization of $\tilde{\varphi}$ so that $\max_{\hat{\mathbf{k}}, \alpha} |\tilde{\varphi}_{\hat{\mathbf{k}}, \alpha}| = 1$. We now take the inner product with the same eigenvector φ and use the orthonormality of the eigenvectors of g to write

$$1 = -\lambda \sum_{\alpha_2} \int_{S_{\alpha_2}} \frac{d\hat{\mathbf{k}}_2}{|S_{\alpha_2}|} |\varphi_{\hat{\mathbf{k}}_2, \alpha_2}|^2 \log \left(\frac{2\omega_c}{\Delta(0) |\tilde{\varphi}_{\hat{\mathbf{k}}_2, \alpha_2}|} \right). \tag{2.102}$$

After rearranging terms, we finally find

$$\Delta(0) = 2\omega_c \exp \left(\frac{1}{\lambda} \right) \exp \left(- \langle \log(|\tilde{\varphi}|) \rangle \right) \tag{2.103}$$

with

$$\langle \log(|\tilde{\varphi}|) \rangle = \sum_{\alpha} \int_{S_{\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\alpha}|} |\varphi_{\hat{\mathbf{k}}, \alpha}|^2 \log(|\tilde{\varphi}_{\hat{\mathbf{k}}, \alpha}|). \tag{2.104}$$

We can then divide by T_c to obtain

$$\frac{2\Delta(0)}{T_c} = 3.53 \exp(-\langle \log(|\tilde{\varphi}|) \rangle) \geq 3.53 \quad (2.105)$$

where 3.53 is the well known BCS value for a uniform gap, and the exponential factor departs from 1 for non-uniform gaps.

2.7.2 Triplet

In the pseudo-spin triplet case, the $\mathcal{H}$ matrix is in general given by

$$\mathcal{H}_{\mathbf{k},\alpha} = \begin{pmatrix} \xi_{\mathbf{k},\alpha} & 0 & -\Delta_{\mathbf{k},\alpha,d_x} + i\Delta_{\mathbf{k},\alpha,d_y} & \Delta_{\mathbf{k},\alpha,d_z} \\ 0 & \xi_{\mathbf{k},\alpha} & \Delta_{\mathbf{k},\alpha,d_z} & \Delta_{\mathbf{k},\alpha,d_x} + i\Delta_{\mathbf{k},\alpha,d_y} \\ -\overline{\Delta_{\mathbf{k},\alpha,d_x}} - i\overline{\Delta_{\mathbf{k},\alpha,d_y}} & \overline{\Delta_{\mathbf{k},\alpha,d_z}} & -\xi_{\mathbf{k},\alpha} & 0 \\ \overline{\Delta_{\mathbf{k},\alpha,d_z}} & \overline{\Delta_{\mathbf{k},\alpha,d_x}} - i\overline{\Delta_{\mathbf{k},\alpha,d_y}} & 0 & -\xi_{\mathbf{k},\alpha} \end{pmatrix}. \quad (2.106)$$

In the following, we will sometimes use the convenient notation $\vec{d} = \Delta_{d_x}\hat{x} + \Delta_{d_y}\hat{y} + \Delta_{d_z}\hat{z}$, where the dependence on $\mathbf{k}, \alpha$ is implicit.

As mentioned before, due to a mirror symmetry present in Sr_2RuO_4 , $\vec{d}$ will always be pointing either out-of-plane ($d_x = d_y = 0$) or in-plane ($d_z = 0$). These states can be called equal-pseudo-spin paired, in analogy with the equal-spin-paired (ESP) states described in Ref. [21].

Let us treat the case of out-of-plane $\vec{d}$ first. Posing $\Delta_{\mathbf{k},\alpha,d_z} \equiv \Delta_{\mathbf{k},\alpha}$, the matrix reads

$$\mathcal{H}_{\mathbf{k},\alpha} = \begin{pmatrix} \xi_{\mathbf{k},\alpha} & 0 & 0 & \Delta_{\mathbf{k},\alpha} \\ 0 & \xi_{\mathbf{k},\alpha} & \Delta_{\mathbf{k},\alpha} & 0 \\ 0 & \overline{\Delta_{\mathbf{k},\alpha}} & -\xi_{\mathbf{k},\alpha} & 0 \\ \overline{\Delta_{\mathbf{k},\alpha}} & 0 & 0 & -\xi_{\mathbf{k},\alpha} \end{pmatrix}. \quad (2.107)$$

It is easily checked that the two blocks lead to the same term in the Hamiltonian. Following the same calculation as for the singlet, we obtain the exact same Hamiltonian as in Eq. 2.112, the same gap equation as in Eq. 2.98, and the same formula for $\Delta(0)$, with d_0 replaced by d_z .

Let us now treat the in-plane $\vec{d}$ case. Once $\vec{d}$ can take different orientations as a function of momentum, one should distinguish between unitary and non-unitary states. A unitary state is such that $\vec{d} \times \vec{d}^* = 0$, a condition which ensures that the state does not have any imbalance between the two (pseudo-)spin species. At zero magnetic field, unitary states are therefore always expected to be favoured over non-unitary ones. For a unitary state with in-plane $\vec{d}$, it is easy to see that one can in full generality always choose a real $\vec{d}$. Posing $\Delta_{\mathbf{k},\alpha} = -\Delta_{\mathbf{k},\alpha,d_x} + i\Delta_{\mathbf{k},\alpha,d_y}$, the Hamiltonian matrix becomes

$$\mathcal{H}_{\mathbf{k},\alpha} = \begin{pmatrix} \xi_{\mathbf{k},\alpha} & 0 & \Delta_{\mathbf{k},\alpha} & 0 \\ 0 & \xi_{\mathbf{k},\alpha} & 0 & -\bar{\Delta}_{\mathbf{k},\alpha} \\ \bar{\Delta}_{\mathbf{k},\alpha} & 0 & -\xi_{\mathbf{k},\alpha} & 0 \\ 0 & -\Delta_{\mathbf{k},\alpha} & 0 & -\xi_{\mathbf{k},\alpha} \end{pmatrix}. \quad (2.108)$$

This time the two blocks lead to two different contributions to the Hamiltonian that are related to each other by time-reversal symmetry.

The Bogolyubov transformation can be written as

$$\begin{aligned} c_{\mathbf{k},\sigma}^\dagger &= v'_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger + v_{\mathbf{k},\sigma}^* b_{\mathbf{k},\sigma} \\ c_{-\mathbf{k},\sigma}^\dagger &= v'_{\mathbf{k},\sigma} b_{\mathbf{k},\sigma}^\dagger - v_{\mathbf{k},\sigma}^* a_{\mathbf{k},\sigma} \end{aligned} \quad (2.109)$$

with

$$\begin{aligned} v'_{\mathbf{k},\sigma} &= i e^{-i\phi_{\mathbf{k},\sigma}/2} \cos(\theta_{\mathbf{k},\sigma}) \\ v_{\mathbf{k},\sigma} &= -i e^{i\phi_{\mathbf{k},\sigma}/2} \sin(\theta_{\mathbf{k},\sigma}) \\ \cot(2\theta_{\mathbf{k},\sigma}) &= \frac{\xi_{\mathbf{k}}}{|\Delta_{\mathbf{k},\sigma}|} \end{aligned} \quad (2.110)$$

where $\Delta_{\mathbf{k},\sigma} = |\Delta_{\mathbf{k},\sigma}| e^{i\phi_{\mathbf{k},\sigma}}$, $\Delta_{\mathbf{k},+} = \Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{k},-} = -\bar{\Delta}_{\mathbf{k}}$. We also give the inverse transformation for later convenience:

$$\begin{aligned} a_{\mathbf{k},\sigma}^\dagger &= (v'_{\mathbf{k},\sigma})^* c_{\mathbf{k},\sigma}^\dagger - v_{\mathbf{k},\sigma}^* c_{-\mathbf{k},\sigma} \\ b_{\mathbf{k},\sigma}^\dagger &= (v'_{\mathbf{k},\sigma})^* c_{-\mathbf{k},\sigma}^\dagger + v_{\mathbf{k},\sigma}^* c_{\mathbf{k},\sigma} \end{aligned} \quad (2.111)$$

with $a_{-\mathbf{k},\sigma}^\dagger = b_{\mathbf{k},\sigma}^\dagger$. Note that the band indices are implicit in all these expressions.

After this Bogolyubov transformation, the Hamiltonian reads

$$\begin{aligned} H_{BCS} &= \frac{1}{2} \sum_{\mathbf{k},\alpha} E_{\mathbf{k},\alpha} (a_{\mathbf{k},\alpha,+}^\dagger a_{\mathbf{k},\alpha,+} + b_{\mathbf{k},\alpha,+}^\dagger b_{\mathbf{k},\alpha,+} + a_{\mathbf{k},\alpha,-}^\dagger a_{\mathbf{k},\alpha,-} + b_{\mathbf{k},\alpha,-}^\dagger b_{\mathbf{k},\alpha,-}) \\ &= \sum_{\mathbf{k},\alpha} E_{\mathbf{k},\alpha} (a_{\mathbf{k},\alpha,+}^\dagger a_{\mathbf{k},\alpha,+} + a_{\mathbf{k},\alpha,-}^\dagger a_{\mathbf{k},\alpha,-}) \end{aligned} \quad (2.112)$$

where $E_{\mathbf{k},\alpha} = \sqrt{\xi_{\mathbf{k},\alpha}^2 + |\Delta_{\mathbf{k},\alpha,+}|^2} = \sqrt{\xi_{\mathbf{k},\alpha}^2 + |\Delta_{\mathbf{k},\alpha,-}|^2}$ and where we omitted the additive constant $\sum_{\mathbf{k},\alpha} (\xi_{\mathbf{k},\alpha} - E_{\mathbf{k},\alpha}) + \bar{\Delta} (V^{BCS})^{-1} \Delta$. The gap equation is again obtained by imposing self-consistency:

$$\begin{aligned}
\Delta_{\mathbf{k}_1, \alpha_1, d_a} &= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_2, \alpha_2, d_b} V_{\mathbf{k}_1, \alpha_1, d_a; \mathbf{k}_2, \alpha_2, d_b}^{BCS} \langle \phi_{\mathbf{k}_2, \alpha_2, d_b} \rangle \\
&= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_2, \alpha_2, d_b} V_{\mathbf{k}_1, \alpha_1, d_a; \mathbf{k}_2, \alpha_2, d_b}^{BCS} \left(\sum_{\sigma} U_{d_b, \sigma \sigma} \langle \phi_{\mathbf{k}_2, \alpha_2, \sigma \sigma} \rangle \right) \\
&= \frac{1}{\sqrt{2}} \sum_{\mathbf{k}_2, \alpha_2, d_b} V_{\mathbf{k}_1, \alpha_1, d_a; \mathbf{k}_2, \alpha_2, d_b}^{BCS} \left(\sum_{\sigma} U_{d_b, \sigma \sigma} (v'_{\mathbf{k}_2, \alpha_2, \sigma})^* v_{\mathbf{k}_2, \alpha_2, \sigma} (1 - 2n(E_{\mathbf{k}_2, \alpha_2})) \right) \\
&= - \sum_{\mathbf{k}_2, \alpha_2, d_b} V_{\mathbf{k}_1, \alpha_1, d_a; \mathbf{k}_2, \alpha_2, d_b}^{BCS} \left(\sum_{\sigma} U_{d_b, \sigma \sigma} \Delta_{\mathbf{k}_2, \alpha_2, \sigma} \right) \frac{\tanh(E_{\mathbf{k}_2, \alpha_2}/2T)}{2E_{\mathbf{k}_2, \alpha_2}} \\
&= - \sum_{\mathbf{k}_2, \alpha_2, d_b} V_{\mathbf{k}_1, \alpha_1, d_a; \mathbf{k}_2, \alpha_2, d_b}^{BCS} \Delta_{\mathbf{k}_2, \alpha_2, d_b} \frac{\tanh(E_{\mathbf{k}_2, \alpha_2}/2T)}{2E_{\mathbf{k}_2, \alpha_2}}
\end{aligned} \tag{2.113}$$

where U is the unitary matrix for the change of basis from $\{(\sigma\sigma') = (++) , (--) \}$ to $\{d_a = d_x, d_y\}$.

The equation for $\Delta(0)$ is the same as in the singlet case:

$$\Delta(0) = 2\omega_c \exp\left(\frac{1}{\lambda}\right) \exp(-\langle \log(|\tilde{\varphi}|) \rangle) \tag{2.114}$$

but with a generalized version of $\langle \log(|\tilde{\varphi}|) \rangle$:

$$\langle \log(|\tilde{\varphi}|) \rangle = \sum_{\alpha} \int_{S_{\alpha}} \frac{d\hat{\mathbf{k}}}{|S_{\alpha}|} \left(|\varphi_{\hat{\mathbf{k}}, \alpha, d_x}|^2 + |\varphi_{\hat{\mathbf{k}}, \alpha, d_y}|^2 \right) \log \left(\sqrt{|\tilde{\varphi}_{\hat{\mathbf{k}}, \alpha, d_x}|^2 + |\tilde{\varphi}_{\hat{\mathbf{k}}, \alpha, d_y}|^2} \right). \tag{2.115}$$

2.7.3 Specific Heat Jump

BCS theory predicts a jump in specific heat ΔC at T_c . The ratio of ΔC to its value in the normal state C_n is a number which, for a clean superconductor in the weak coupling limit, depends only on the momentum-space anisotropy of the gap. For a gap norm given at the Fermi surface by $|\Delta_{\hat{\mathbf{k}}, \alpha}| = \Delta |f_{\hat{\mathbf{k}}, \alpha}|$, where Δ is a positive constant, this ratio is given by [20, 22]

$$\frac{\Delta C}{C_n}(T_c) = \frac{12}{7\zeta(3)} \frac{\langle |f_{\hat{\mathbf{k}}, \alpha}|^2 \rangle_{\text{FS}}^2}{\langle |f_{\hat{\mathbf{k}}, \alpha}|^4 \rangle_{\text{FS}}} \tag{2.116}$$

where

$$\langle h_{\mathbf{k}, \alpha} \rangle_{\text{FS}} = \frac{1}{\rho} \sum_{\alpha} \int_{\text{FS}_{\alpha}} \frac{d\hat{\mathbf{k}}}{(2\pi)^D} \frac{1}{v_{\mathbf{k}, \alpha}} h_{\mathbf{k}, \alpha}, \tag{2.117}$$

where $\frac{12}{7\zeta(3)} \simeq 1.43$, where ρ is the total density of states at the Fermi level and where

$$|f_{\hat{\mathbf{k}},\alpha}| = \sqrt{\sum_{d_\mu} |\tilde{\varphi}_{\mathbf{k},\alpha,d_\mu}|^2}. \quad (2.118)$$

One can easily insert the gap functions predicted in the previous sections in this formula to obtain a prediction for $\frac{\Delta C}{C_n}$ and compare it with experiments. This will be used in Chap. 3 for the case of Sr_2RuO_4 .

2.8 Conclusion

We give here a summary of the main results established in this Chapter. Given a multi-orbital hopping model describing a metal and an interaction Hamiltonian, one can study the onset of superconductivity in the infinitely small interaction limit by the following procedure. First, diagonalize the single-particle Hamiltonian, define a momentum-dependent pseudo-spin basis if spin-orbit coupling is present, and locate the Fermi surfaces for the different bands, $\{\hat{\mathbf{k}}, \alpha\}$. Second, compute and diagonalize the pairing matrix $g_{\hat{\mathbf{k}}_1,\alpha_1,d_{\mu_1};\hat{\mathbf{k}}_2,\alpha_2,d_{\mu_2}}$, where d_0 gives the pseudo-spin singlet sector, and $d_{x,y,z}$ give the pseudo-spin triplet sector. The eigenequation is given by

$$\sum_{\alpha} \sum_{d_\mu} \int_{S_\alpha} \frac{d\hat{\mathbf{k}}}{|S_\alpha|} g_{\hat{\mathbf{k}}_1,\alpha_1,d_{\mu_1};\hat{\mathbf{k}},\alpha,d_\mu} \varphi_{\hat{\mathbf{k}},\alpha,d_\mu} = \lambda \varphi_{\hat{\mathbf{k}}_1,\alpha_1,d_{\mu_1}}. \quad (2.119)$$

The pairing matrix is directly related to the 2-particle irreducible effective vertex in the Cooper channel calculated at leading order in U/t :

$$g_{\hat{\mathbf{k}}_1,\alpha_1,d_{\mu_1};\hat{\mathbf{k}}_2,\alpha_2,d_{\mu_2}} \equiv \sqrt{\rho_{\alpha_1} \frac{\bar{v}_{\alpha_1}}{v_{\hat{\mathbf{k}}_1,\alpha_1}}} \Gamma_{\hat{\mathbf{k}}_1,\alpha_1,d_{\mu_1};\hat{\mathbf{k}}_2,\alpha_2,d_{\mu_2}} \sqrt{\rho_{\alpha_2} \frac{\bar{v}_{\alpha_2}}{v_{\hat{\mathbf{k}}_2,\alpha_2}}}. \quad (2.120)$$

After discretization of the Fermi surfaces, $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$ only take a finite number of values, and g becomes a hermitian matrix that is easily diagonalized numerically. The most negative eigenvalue λ gives the most favored superconducting order parameter, with a critical temperature given by $T_c \propto e^{1/\lambda}$ and an order parameter functional form given by the corresponding eigenvector. One can then study the superconducting phase by using a BCS mean-field Hamiltonian where the gap functional form is assumed independent of T .

2.8.1 Range of Validity

The discussion in this Chapter is valid as long as the non-interacting particle-hole susceptibility χ^{ph} is non-divergent. If χ^{ph} diverges, instabilities different from BCS can appear even in the weak coupling limit and the assumption of BCS being the only instability therefore breaks down. This is always the case in one dimension, where χ has a divergence at $2k_F$ because of the perfect nesting of the Fermi surface given by two points at $\pm k_F$. In this case, there is competition between the BCS instability and the charge-density wave instability. They actually exactly cancel each other so that fermions in 1D form a Luttinger liquid that remains gapless even in the presence of interactions [5, 23, 24]. A divergent non-interacting particle-hole susceptibility can also occur in 2D at a Van Hove singularity [25], but requires fine-tuning of the hoppings and of the electron density. A Van Hove singularity is a divergence of the density of states that arises when the chemical potential goes through an extremum or a saddle-point of the dispersion relation. We will discuss the evolution of the superconducting state in Sr_2RuO_4 across such as a Van Hove singularity in Chap. 5. While for a strictly two-dimensional system the weak coupling analysis breaks down strictly at the Van Hove point, it is still valid arbitrarily close to it, as long as the interaction is small enough. Furthermore, if one actually takes into account the inter-layer coupling in Sr_2RuO_4 , one obtains a 3D system for which the density of states does not diverge at a Van Hove point (only its derivative does) [25].

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