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**Using a flux threaded composite loop to
identify the pairing symmetry of iron
based superconductors**

Rosa Rodríguez Mota

Department of Physics

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McGill University, Montreal

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Abstract

Identifying the correct order parameter structure of the iron based superconductors family will provide insight about the pairing mechanism in these materials. Due to their multi-orbital band structure, the proximity of the superconducting phase to an anti-ferromagnetic phase, and the fact that superconductivity on these materials is associated to the Fe-pnictide layer, most theories favour an unconventional pairing mechanism, and an $s_{\pm}$ pairing symmetry, which changes signs between the electron and hole Fermi pockets. However, as most experiments are only sensitive to the magnitude of the order parameter and theoretical proposals for phase sensitive experiments are challenging, the $s_{\pm}$ structure remains unconfirmed. In 2010, Chen *et al.* performed a phase sensitive experiment that showed evidence of integer flux quantum and half integer flux quantum jumps in a Nb-NdFeAsO_{0.88}F_{0.12} composite loop [1]. This experiment has been interpreted as evidence of the predicted $s_{\pm}$ pairing symmetry. Inspired by these results, we present a microscopic lattice model to study the energy dependence on flux for an iron-pnictide/ s -wave superconductor composite loop.

Résumé

Identifier la structure du paramètre d'ordre de la famille de supraconducteurs à base de fer permettrait de mieux comprendre le mécanisme de création de paires dans ces matériaux. En raison de leur structure de bande multi-orbitale, de la proximité entre leur phase supraconductrice et anti-ferromagnétique ainsi que de la relation entre la supraconductivité et la couche Fe-pnictide qui leur est propre, la plupart des théories favorisent pour ces matériaux un mécanisme de formation de paires non-conventionnel. Les modèles théoriques prévoient également une symétrie $s_{\pm}$ dans la formation des paires, qui change de signe entre les électrons et les trous dans la surface de Fermi. Néanmoins, puisque les expériences actuelles ne sont sensibles qu'à la grandeur du paramètre d'ordre, la structure $s_{\pm}$ reste à confirmer. En 2010, Chen *et al.* ont exécuté une expérience sensible à la phase ayant montré l'existence de transitions de multiples entiers et demi-entiers de quantum de flux entier dans une boucle composite de Nb-NdFeAsO_{0.88}F_{0.12} [1]. Cette expérience a été interprétée comme une évidence de la symétrie $s_{\pm}$ dans la formation de paires. Inspirées par ces résultats, nous présentons un modèle de réseau microscopique pour étudier la dépendance en flux de l'énergie dans une boucle composite supraconductrice de fer-pnictide et un supraconducteur s sphérique.

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Introduction

The antagonistic relation between ferromagnetism and superconductivity can be easily exemplified by considering the response of a ferromagnet and a superconductor to a magnetic field. In the presence of such a field, a ferromagnet tends to concentrate the field while a superconductor tends to expel it. Therefore, it was the general belief that a strongly magnetic element, such as iron, was not a good building block for a superconductor. This belief was proven to be erroneous when in 2006 [6] superconductivity in an iron-based material (LaOFeP) with a transition temperature (T_c) of 4 K was first reported. However it was not until February 2008, that the same research group discovered 26 K superconductivity in fluorine-doped LaFeAsO [7], and this new type of superconductor gained worldwide attention. Through the continued work of many physicists, LaFeAsO was quickly joined by over 50 similar superconductors whose critical temperatures would go as high as 56 K [8] [9]. This made this family a candidate for high T_c superconductivity, which for 22 years seemed to be exclusive to the cuprate superconductors. Since their unexpected discovery, iron based superconductors have challenged the previous set of paradigms on superconductivity and motivated us to improve our understanding of the origins of this phenomenon.

The similarities and differences between the iron-pnictides and the cuprates have been established from the beginning. Among the similarities we can find: both types of su-

perconductor are layered materials, the superconducting phase in both cases is close to an antiferromagnetic phase, and doping through chemical substitution plays a key role in obtaining the superconducting phase. The phase diagram of the iron-pnictides also resembles those of other unconventional superconductors, such as the heavy fermion and organic superconductors. These considerations, together with other characteristics which will be discussed later, lead us to believe that the nature of the pairing mechanism in these systems is indeed unconventional. This belief gives us strong motivation to study them since they could provide important insights that would help in deciphering the puzzle of unconventional superconductivity.

There are several key differences between the iron based superconductor and the high T_c cuprates. These differences will be marked throughout this introduction, but we mention them briefly here. We will start by noting that the layer in which superconductivity occurs (active layer) in the iron pnictides is corrugated as opposed to the planar CuO_2 layers of the cuprates. Another difference is that the cuprate parent compounds are Mott insulators, whereas the iron based superconductors parent compounds are metallic; this makes the iron based superconductors more manageable for applications. Also, superconductivity in the cuprates is destroyed when doping in the CuO_2 active layers, while in the iron based superconductors doping in the active layer does not destroy superconductivity. Finally, there are many iron based compounds that show coexistence of superconductivity with long range magnetic order. With the exception of some cases, perhaps disorder induced [10], the cuprates do not exhibit this coexistence.

Although the iron based superconductors are generally compared with the cuprates, some of their characteristics set them very close to the heavy fermion superconductors. Like the cuprates and the iron pnictides, the heavy fermion superconductors are also layered materials whose phase diagram exhibits a magnetically ordered phase as well as a superconducting phase. The heavy fermion systems are metallic as the iron pnictides in

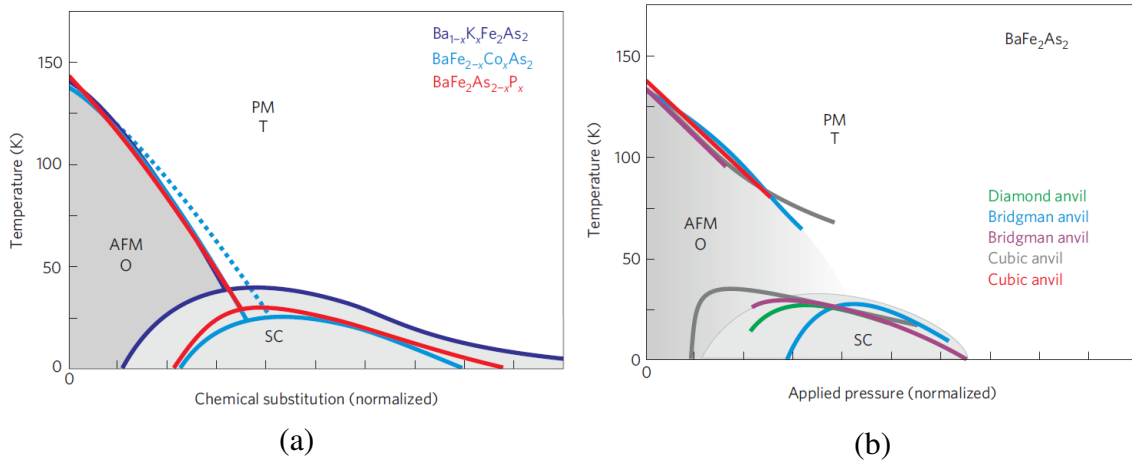


Figure 1.1: Compilation of experimental phase diagrams for BaFe_2As_2 showing superconducting (SC), antiferromagnetic (AF), paramagnetic (PM), tetragonal (T) and orthorhombic (O) phases. (a) Phase diagram of BaFe_2As_2 for chemical substitution with K, Co and P. The dotted line indicates the transition between the tetragonal and the orthorhombic phase. (b) Phase diagram of BaFe_2As_2 as a function of applied pressure using several techniques. In both (a) and (b) the amount of chemical substitution and the applied pressure are normalized to overlap the descent of the AFM phase to simplify comparison. Reprinted by permission from Macmillan Publishers Ltd: [Nature] [2], copyright (2010).

their normal phase. They also exhibit coexistence of superconductivity and antiferromagnetic order.

The superconducting phase in iron based compounds can be tuned either by doping through chemical substitution or by applying pressure. In Figure 1.1 we can see a compilation of experimental phase diagrams for the compound BaFe_2As_2 . This compound is one of the most studied members of the iron based superconductors family, and the compilation shown in Figure 1.1 contains many of the distinctive features of the family. Besides the superconducting transition and magnetic transitions, the iron based compounds also undergo a structural transition between an orthorhombic phase and a tetragonal phase. The phase diagram of all iron based compounds shows an antiferromagnetic phase and a superconducting phase, but the qualitative behaviour of the phase diagram varies. There are compounds where these phases are separated as a function of doping and do not overlap, while the phase diagram of others shows coexistence of superconductivity and magnetic

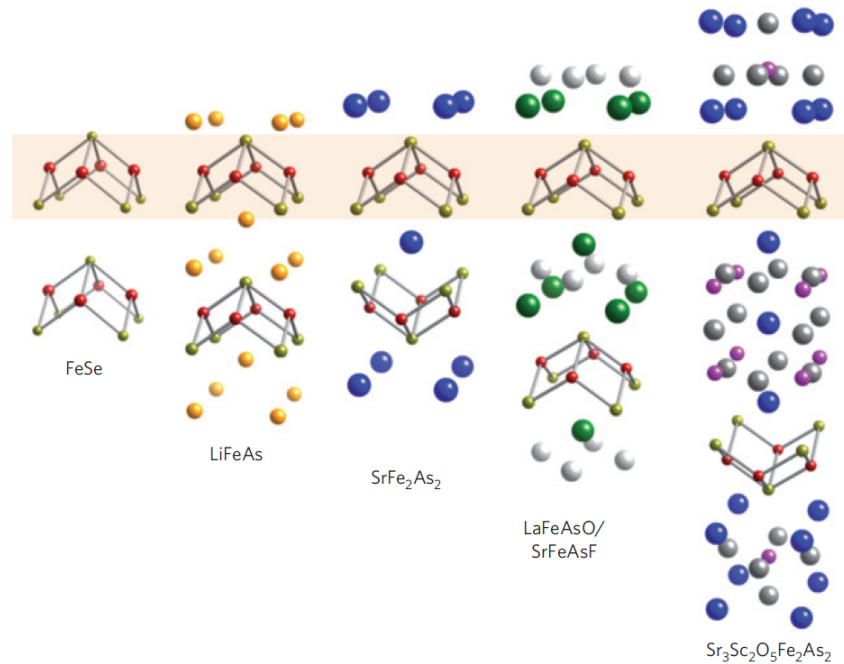


Figure 1.2: Five out of the six structures of iron based compounds known to support superconductivity. From left to right, each compound represents the families: 11, 111, 122, 1111, and 32522. The shared Fe-pnictogen(or chalcogen) layer is highlighted in red, the red ions in this layer are iron and the yellow ones pnictogen (or chalcogen). The largest transition temperatures belong to members of the 1111 family. Reprinted by permission from Macmillan Publishers Ltd: [Nature] [2], copyright (2010).

ordering, see [11] for examples.

1.1 Crystal structure

To this day, six different structural families of iron-based superconductors (11, 111, 122, 1111, 3255 and 42622) have been found. Figure 1.2 displays five of them. All of these structures consist of layers made of iron and a pnictogen (P or As), or a chalcogen (S, Se, Te) in the case of the 11 family, arranged on a stacked sequence separated by “blocking layers”, or without “blocking layer” in the 11 family, that can be composed of alkali, alkali-earth, rare-earth oxide or fluoride, or even more complicated perovskite-type combinations as in the 32522 and the 42622 family. The general consensus is that the superconducting

electrons live in the Fe-pnictogen common layers analogously to the copper-oxygen layers of the cuprate superconductors. However, in the superconducting layers of the iron based superconductors the pnictogen anions are located above and below the iron plane in contrast to the planar copper-oxygen structure of the cuprates.

That structural difference between the iron-pnictides and the cuprates leads to a very different electronic structure. The valence electrons of both Fe and Cu occupy $3d$ orbitals. Since the Fe-pnictogen layer of the iron based superconductors is not planar, the Fe ions are closer to each other than the Cu ions in a cuprate superconductor. The Fe ions' closer packing results in all five Fe $3d$ orbitals contributing to the density of states near the Fermi surface. In contrast, the cuprates can be well described considering only one Cu $3d$ orbital.

1.2 Multi-band structure

The band structure of the iron based superconductors is complex, with all of the Fe $3d$ orbitals ($3d_{z^2}$, $3d_{x^2-y^2}$, $3d_{xy}$, $3d_{xz}$, $3d_{yz}$) making a contribution close to the Fermi energy. These orbitals hybridize among themselves and through the pnictogen p orbitals. Since superconductivity arises due to an instability on the Fermi surface, studying the shape of the Fermi surface and the band structure near it is a key step in understanding the superconducting phase of the material. Many authors have calculated the band structure of several iron based superconductors from first principles density functional theory (DFT). In Figure 1.3 the band structure and Fermi surface of LaOFeP [3] are shown. From 2 eV below the Fermi energy to 2 eV above the Fermi energy, we can find contribution of all five $3d$ Fe orbitals. The Fermi surface of LaOFeP is formed by five sheets: four of them are quasi-cylindrical parallel to the k_z direction, and the fifth one is a 3D heavy hole pocket derived from the $3d_{z^2}$ orbital which hybridizes sufficiently with the p orbitals to yield a 3D contribution. The rest of the sheets are almost 2D. They consist of two electron pockets located

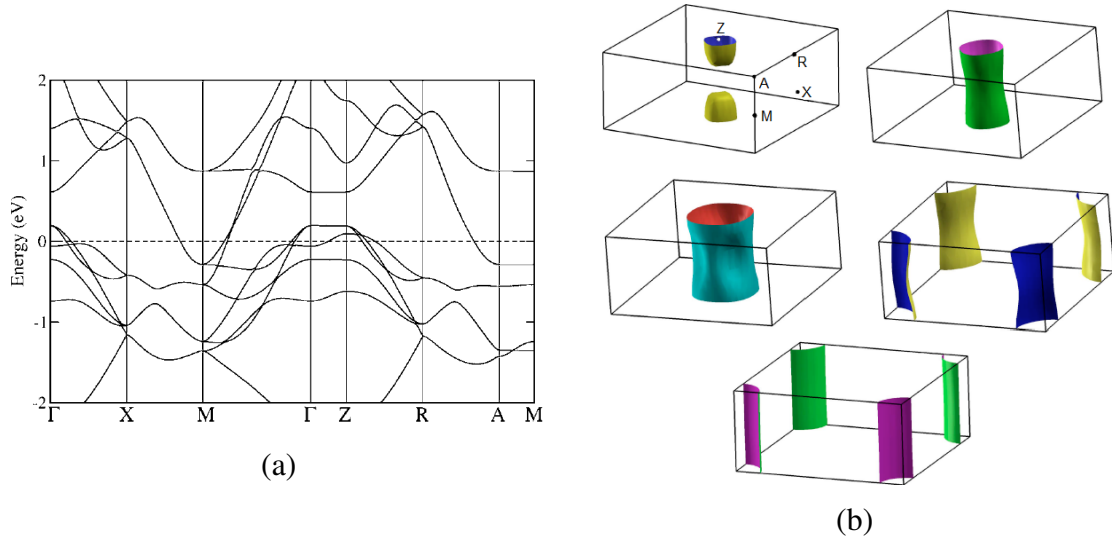


Figure 1.3: (a) Band structure LaOFeP derived from first principles calculations. The Fermi energy is set at 0 eV. (b) Fermi surface for LaOFeP in the Brillouin zone with center at the Γ point. Adapted from [3] Copyright (2007) by The American Physical Society

around the M point and two hole pockets located around the Γ point. Other members of the iron based superconductors family share similar Fermi surfaces, with the exception of the 3D heavy hole pocket [12], which seems to be very sensitive to structural details and is absent in many iron based superconductors.

As noted by D.J. Singh and M.-H. Du [13], the electron pockets have higher velocities than the hole pockets. The electron pockets are associated with the in plane Fe (d_{xy} , $d_{x^2-y^2}$) orbitals and will make the larger contribution to the in plane electrical conductivity. Also, these materials should be characterized as low carrier density, high density of states metals, near itinerant magnetism. This differs from the cuprates which have high carrier density and a lower density of states than the pnictides, setting them far from itinerant magnetism.

It has been widely documented that this electronic structure is unstable to both magnetic ordering and superconducting pairing. We can illustrate this by considering the case in which one of the electron Fermi surface sheets has roughly the same area as one of the hole Fermi surface sheets. If this were the case, since one sheet is located at the center of the zone and another one at the corner, a magnetic order vector joining the M and the Γ points

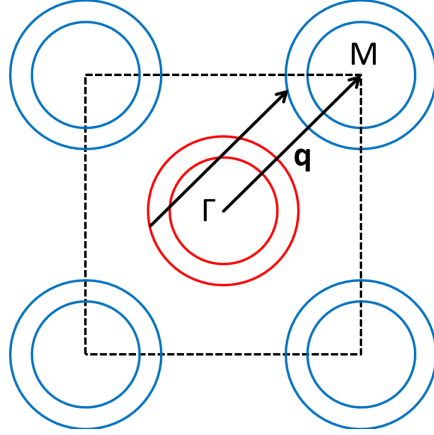


Figure 1.4: Nesting instability of the Fermi surface of iron based superconductors. The image shows a 2-D representation of the quasi-cylindrical sheets of the Fermi surface of iron based superconductors, the hole pockets are represented in red, the electron pockets, in blue, and the Brillouin zone is enclosed by the dashed square. A magnetic vector $\mathbf{q}$ joining the M and the Γ points of the Fermi surface nests a circle of points on each of two different Fermi surface sheets. In a more realistic scenario, this nesting is not exact.

(π, π) would nest a circle of points on each of the two different Fermi surface sheets. This nesting, shown in Figure 1.4, will result in enhanced spin fluctuations at the nesting vector which, if strong enough, may lead to a spin-density wave [12]. Such SDW has been found in undoped iron-pnictides in first principles calculations [13] as well as experimentally [14].

This basic Fermi surface structure, consisting in hole pockets around the M point and electron pockets around the Γ point, has been confirmed by several angle-resolved photoemission spectroscopy (ARPES) measurements [15] [16] [17] [18]. Additionally, ARPES measurements show that the effects of electron and hole doping are well captured by changing the chemical potential in a rigid structure band, showing that the topology of the Fermi surface is maintained in both scenarios. As a consequence of hole doping, the hole pocket increases in size and the electron pocket contracts [19]. Meanwhile, the measured effect of electron doping is the opposite with the hole pocket decreasing and the electron pocket expanding [20].

1.3 Itinerant vs localized magnetism

As most evidence points towards the mechanism that leads to superconductivity in the iron based superconductors being the same as the one leading to the AFM order, much effort has been put towards trying to elucidate the origin of the magnetic interactions in these systems. All iron pnictides undergo an antiferromagnetic transition, and even though the nature of this transition is different for each compound, they all share an antiferromagnetic order, shown in Figure 1.5, consisting of antiferromagnetic stripes in one direction of the Fe lattice and ferromagnetic stripes in the other. The AFM phase of the members of the 11 family has a different ordering in which there are two lines of aligned spins instead of just one [21], although it is important to point out that experimentally all 11 compounds are synthesized with excess Fe.

The nature of magnetism in the iron based superconductors is an extremely controversial topic, and there are two opposing views. At first glance, it seems that the magnetic order originates from the Fermi surface nesting between itinerant electrons [13], which could induce a spin density wave consistent with Figure 1.5. However, this ordering is also consistent with a localized antiferromagnetic exchange $J_1 - J_2$ with nearest neighbours J_1 and next nearest neighbours J_2 coupling satisfying $J_1 < 2J_2$. Furthermore, there are reasons to believe that electron-electron correlations may be sufficiently strong to make local moments have important contributions to the magnetic and superconducting properties of these materials [22] [23] [24]. The itinerant view of magnetism in the iron based superconductors is consistent with weak coupling, and the localized view, with strong coupling. Therefore, to ask whether the magnetic behaviour in these materials is itinerant or localized is equivalent to ask whether the interactions in them are weak or strong.

Most models supporting the itinerant view of the magnetic properties in iron based compounds focus on the spin density wave nesting of the Fermi surface. Also, the high density of states at the Fermi surface sets them close to a Stoner instability. In general,

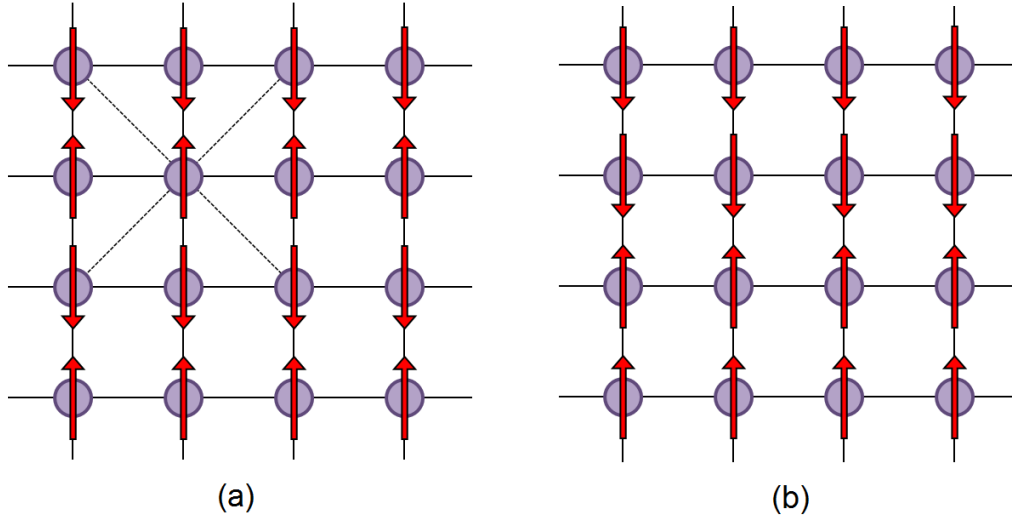


Figure 1.5: (a) AFM ordering found in all iron based compounds except for the 11 family. The spins of all next-nearest neighbours are anti-aligned which is consistent with a J_1 - J_2 antiferromagnetic coupling with $2J_2 > J_1$. (b) AFM ordering found in the 11 family.

the qualitative nature of the magnetic behaviour is well predicted by density functional calculations, however, there are serious quantitative problems with this scenario. In particular, density functional calculations using real cell parameters tend to predict a much larger magnetic momentum than measured by neutron scattering experiments [25]. Furthermore, members of the 11 family share the same Fermi surface structure, but they have a different magnetic ordering, which is inconsistent with magnetism purely arising from the Fermi surface nesting.

The clearly metallic nature of the iron pnictide parent compounds is, at least in principle, incompatible with a localized exchange model. Nevertheless, despite being metallic most of these compounds have a strikingly high resistivity. Thus it is worth considering the scenario in which they are close to a Mott insulator. If this were the case, it would be appropriate to describe the system via localized spin interactions. Local moment models explain the small magnetic moment of the parent compounds through magnetic frustration[24]. Moreover, Heisenberg models can be phenomenologically fitted reasonably well to some

experimental results [26]. Calculations of the As bridged superexchange interactions [27] [28] show that the exchange between nearest neighbours and next nearest neighbours are both antiferromagnetic and have comparable strength, with $2J_2 > J_1$. But the validity of these calculations is questionable since the direct overlap of the Fe orbitals in the iron pnictides is large enhancing the nearest neighbour antiferromagnetic exchange, and the Hubbard U in the pnictides is not large enough to justify the introduction of a $J_1 - J_2$ model [29]. Furthermore, there is no real evidence of proximity to a Mott transition in the iron pnictides.

Owing to the evidence presented above, it can be concluded that the iron pnictides do not fit simply into an either weak or strong coupling limit [22]. This has led authors to propose models which are not purely localized or purely itinerant. For example, Johannes and Mazin [30] propose to consider the origin of magnetism in these compounds being due to large local Hund's rule coupling and the ground state being selected by itinerant, essentially single-electron, interactions. Another example is the work of Yin, Lee, and Ku [31] who use a model consisting of both itinerant electrons and localized spins from which they can derive the two different behaviours shown in Figure 1.5.

Besides the controversial nature of magnetic interactions in the iron-based superconductors, the development of a microscopic theory of magnetism in these compounds gets further complicated by its multi-band electronic structure. Therefore, further experimental and theoretical research is needed to understand magnetic phenomena in the iron-pnictides.

Despite the controversy on the description of magnetic interaction in these materials, the pairing symmetry predicted by weak itinerant coupling [32] is the same as the one predicted by a strong localized exchange [5]. This pairing symmetry ($s_{\pm}$) consists of an order parameter which changes sign between the electron and hole pockets of the Fermi surface. These results are not surprising because most models used for the iron pnictides consist of a Fermi surface with one or more electron pockets and one or more hole pockets displaced by

a spin density wave vector $(\pi,0)$ in the Fe Brillouin zone. Whether they consider that spin fluctuations originate from Fermi surface nesting or $J_1 - J_2$ exchange, the spin fluctuations will lead to the same sign changing order parameter as long as the leading pairing agent is considered to have the same wave vector. Details of the models and the inclusion of other spin fluctuations will affect the gap magnitudes on the different sheets or the isotropy of the order parameter, but, for a realistic choice of parameters, they are unlikely to change the $s_{\pm}$ symmetry [29].

1.4 Other pairing mechanisms

Although most of the current evidence in iron based superconductors points towards Cooper pairing driven by magnetic fluctuations, we still need to consider other possible pairing mechanisms. To begin this discussion, we start by mentioning that the conventional pairing mechanism, electron phonon coupling, seems to be too weak to account for the relatively large critical temperature of the iron pnictides. While magnetic effects increase the electron phonon coupling parameter, calculations taking it into consideration still give a coupling parameter small enough to rule out electron phonon interaction as the main pairing mechanism [33]. This is also true for experimental determinations of the phonon-coupling parameter [34]. However, there are experiments which measure an isotope effect, although only for Fe substitution, suggesting that phonon modes related to the Fe may play a role in the superconductivity. Once again there is some controversy about these results, with some authors finding a positive isotope effect and others a negative one [11]. Hence, the role that electron-phonon coupling plays in iron based compounds is not entirely determined. Nevertheless, according to the current experimental evidence it does not seem to be the main pairing mechanism. Another possible pairing mechanism that has not received

much attention is charge fluctuations. This mechanism was proposed unsuccessfully for the cuprates and MgB_2 . In the iron pnictides, the lattice stability makes this pairing mechanism unlikely [29]. Finally, we ought to mention that the roles played by correlations and quantum criticality in the iron based superconductors still need to be clarified [2].

1.5 Experimental determination of the pairing symmetry

Currently, the nature of the fundamental mechanism that leads to superconductivity in iron based superconductors is unknown and most evidence points towards an unconventional mechanism. A successful experimental determination of the pairing symmetry would give a definite answer to whether the iron-based superconductors are conventional or not. It would also be of great use in narrowing down possible microscopic theories of the origin of superconductivity in these compounds. This is why many experiments whose objective is to determine the pairing symmetry have been and are being carried out.

In relation to the symmetry of the order parameter, the first question that arises is whether the superconducting state is singlet or triplet. Fortunately, we can say with relatively good confidence that the parity of the superconducting state is singlet. This is shown by Knight shift measurements in NMR experiments performed in members of different families of the iron-based superconductors [35] [36] [37]. The fact that the superconducting state is singlet means that the symmetry of the order parameter must be even. Since the symmetry of the order parameter must also be compatible with the tetragonal symmetry of the lattice, we are left with three possible options: conventional s -wave symmetry, d -wave symmetry and the much discussed $s_{\pm}$ symmetry.

Determining the orbital symmetry of the order parameter has proven to be far more challenging, and it is the focus of ongoing research. We can roughly divide the experiments that probe the symmetry of the order parameter into two groups: (1) experiments that probe

its amplitude, and (2) experiments that probe its phase.

1.5.1 Amplitude sensitive experiments

Experiments that probe the order parameter amplitude are relatively easy to perform and are sensitive to the presence of nodes and multiple gaps in the order parameter. One of these probes is ARPES. In the iron pnictides, ARPES measurements are generally consistent with a fully gapped behaviour. Another way to detect the presence of nodes in a superconductor is through thermodynamic measurements, such as the temperature or magnetic field dependence of the specific heat, NMR relaxation time, London penetration depth and thermal conductivity. In a nodeless superconductor most thermodynamic quantities are exponentially activated with temperature, i.e. are proportional to $\exp(-\Delta/T)$. Any deviation from this exponentially activated behaviour is an indication for the presence of nodes. In the iron based superconductors, the results found from thermodynamic measurements are varied and contradictory. The reasons for this contradictions vary from trivial reasons, such as the quality of the samples, to more subtle and important reasons, such as the complicated structure of the Fermi surface and the multiple bands. Overall, there are some iron compounds that are more or less consistent with nodal behaviour, LaFePO , KFe_2As_2 , P doped BaFe_2As_2 and overdoped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$, while others, such as $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and underdoped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ are mostly consistent with fully gapped behaviour [11].

1.5.2 Phase sensitive experiments

In view of the controversial results of the amplitude sensitive experiments and the difficulty of fully determining the symmetry of the order parameter from them, it is extremely important to perform phase sensitive experiments. In the cuprates, the unambiguous identification of the pairing symmetry as d -wave came primarily from phase sensitive experiments. In order to give an idea of what we mean by phase sensitive experiments, we begin with a

short section in which we discuss some of the experiments that give evidence of a d -wave order in the cuprate superconductors, before going into the discussion of phase sensitive experiment in iron based superconductors.

Phase sensitive experiments in cuprate superconductors

In general, phase sensitive experiments in cuprate superconductors consist of obtaining a π shift in Josephson junctions. Due to the d -wave symmetry of the order parameter such π shift is guaranteed to happen for junctions with certain structures. An example of this type of experiment is the measurement of a π shift in a dc SQUID between a d -wave and an s -wave superconductor constructed, as shown in Figure 1.6 [38]. The d -wave superconductor is oriented so that one of the junctions is along the crystallographic direction a , and the other one, along the crystallographic direction b . Since the phase coherence must be maintained around the loop, we must have:

$$\Phi_a - \Phi_b + 2\pi\Phi/\Phi_0 + \delta_{ab} = 2\pi n \quad (1.5.1)$$

In the above equation, Φ_a, Φ_b are the gauge invariant phase shifts across the junctions, Φ the magnetic flux, Φ_0 the superconducting flux quantum, and n is an integer number. The term δ_{ab} is the internal phase difference between pairs tunnelling across the two junctions. For d -wave symmetry with the chosen orientation of the crystal, the internal phase shift δ_{ab} is equal to π . In the absence of current, $\Phi_a - \Phi_b = 0$, therefore, the constraint given by equation (1.5.1) becomes $\Phi = (n - 1/2)\Phi_0$. This means that the ground state of the junction will be given by half integer values of flux quantum. If the junction were made with two s -wave superconductors, then the phase shift δ_{ab} would be zero and the ground state of the junction would be given by integer values of flux quantum. This distinction allows us to use the experiment to distinguish between s -wave symmetry and d -wave symmetry.

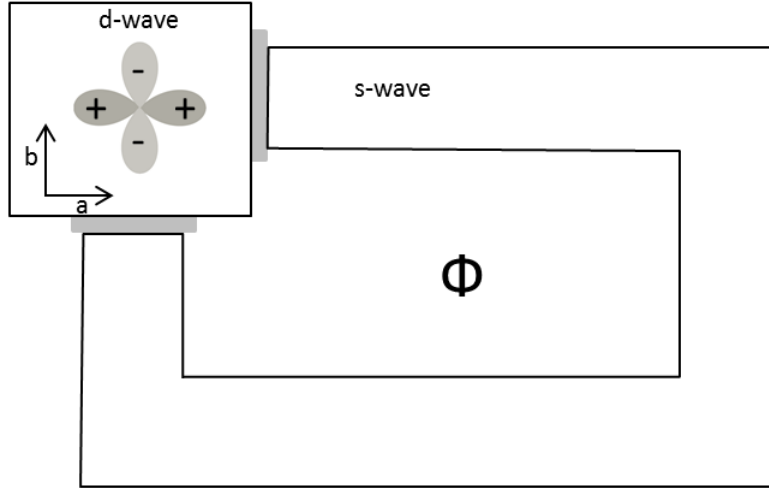


Figure 1.6: Scheme of a π -junction made from a corner junction between a *d*-wave superconductor and an *s*-wave superconductor threaded by the flux Φ . The *d*-wave superconductor must be oriented so that the crystallographic directions *a* and *b* are in the direction of the junctions.

Following this general idea, there are many different ways in which the internal phase difference in *d*-wave superconductors can be exploited to cause a π shift in Josephson junctions. Such π shift have been measured in corner junctions [39] and zig zag junctions [40] between an *s*-wave and a *d*-wave superconductor, and tricrystal grain junctions between three *d*-wave superconductors [41], among others. Because of these experiments, the pairing symmetry of the cuprate superconductors has been successfully identified as *d*-wave.

Phase sensitive experiments in the iron based superconductors

There are several theoretical proposals for tunnelling and SQUID experiments capable of distinguishing between *s*-wave and $s_{\pm}$ symmetry [42] [43] [44] [45]. All these proposals require junction geometries considerably more difficult to prepare than a corner junction, and because of this, no experimental results have been yet reported. Despite these difficulties, there has been some progress made by phase sensitive experiments. First, the absence of half-integer flux in a scanning SQUID experiment [46] and, the measurement of

a Josephson current along the direction of the crystallographic structure in which the layers are stacked [47], provide strong evidence against d -wave pairing. Secondly, two phase sensitive experiments whose results seem to favour the $s_{\pm}$ symmetry have been made.

The first of these experiments, performed in 2010 by Chen *et al.*, consists of a composite loop made of Niobium and $\text{NdFeAsO}_{0.88}\text{F}_{0.12}$ excited with electromagnetic pulses. After a pulse passes, the flux in the loop relaxes back to zero flux. By measuring how the flux inside the loop evolves with time during this relaxation, Chen *et al.*, were able to see that the flux inside the loop can change in both integer and half-integer flux quantum jumps [1]. The half integer jumps are interpreted as arising from a phase shift of π in tunnelling at the Nb- $\text{NdFeAsO}_{0.88}\text{F}_{0.12}$ interface, which as shown by [43] [44] may occur if the $\text{NdFeAsO}_{0.88}\text{F}_{0.12}$ order parameter has sign-changing $s_{\pm}$ symmetry. These results are completely incompatible with a conventional s -wave symmetry. As the d -wave symmetry was ruled out by the previous mentioned experiments, Chen *et al.* results favour the $s_{\pm}$ pairing symmetry. Since this experiment is a central part of this thesis we will describe it with more detail in the next section.

The other phase sensitive experiment that provides evidence in favour of the $s_{\pm}$ symmetry uses spectroscopic-imaging scanning tunnelling microscopy (SI-STM) to measure the quasi-particle scattering strength dependence of magnetic field in $\text{Fe}(\text{Se},\text{Te})$ [4]. Impurities, always present in samples, cause scattering and interference between the quasi-particles. The quasi-particle interference (QPI) can be obtained by taking the Fourier transform of the spectroscopic image [48] [49]. QPI measurements can give information on the quasi-particle states and on the relative sign of the order parameter.

At low enough energies, the QPI is dominated by quasi-particle scattering vectors $\mathbf{q}$ that connect different $\mathbf{k}$ points on the Fermi surface. In the iron based superconductors, since the Fermi surface is formed by multiple pockets, the dominant $\mathbf{q}$ vectors may connect points in different pockets. If the order parameter is $s_{\pm}$ the inter-pocket transitions may

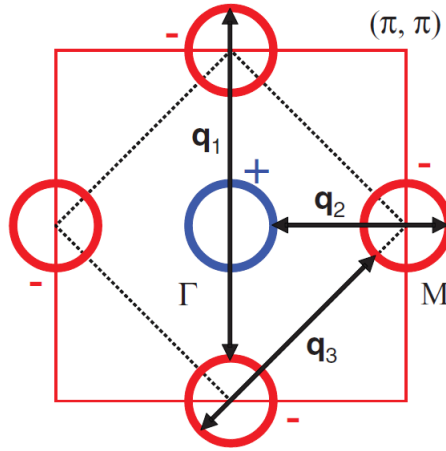


Figure 1.7: Fermi surface and dominant $\mathbf{q}$ scattering processes. The red square indicates the unfolded Brillouin zone, while the dotted diamond, the crystallographic Brillouin zone. For simplicity, the two electron cylinders around Γ are represented by one circle, and so are the two hole cylinders around M . The scattering vectors $\mathbf{q}_2$ and $\mathbf{q}_3$ connect sets of Fermi points in different pockets and $\mathbf{q}_1$ gives umklapp processes. From [4]. Reprinted with permission from AAAS.

occur between $\mathbf{k}$ points where the order parameter has different signs. In Figure 1.7, we can see three different dominant vectors: $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$. The scattering vector $\mathbf{q}_1$ represents intra-pocket umklapp scattering; the processes with scattering vector $\mathbf{q}_2$ change the order parameter's sign; and the ones whose scattering vector is $\mathbf{q}_3$ are inter-pocket scattering processes that preserve the sign of the order parameter.

The effect of the sign changing order parameter in the QPI depends strongly on the nature of the impurity that causes the scattering process. For a non-magnetic impurity the effect of the sign change is to suppress the scattering at $\mathbf{q}$ processes that join points on the Fermi surface with the same order parameter's sign. For a magnetic impurity the effect of the sign change is exactly the opposite: the scattering processes between $\mathbf{k}$ points with different order parameter's sign are suppressed. The QPI dependence on the sign change can be used to probe the order parameter symmetry. However, in a real sample, different scatterers coexist making it difficult to distinguish the previously mentioned effects. Nevertheless, this difficulty can be overcome by introducing vortices as additional sources of

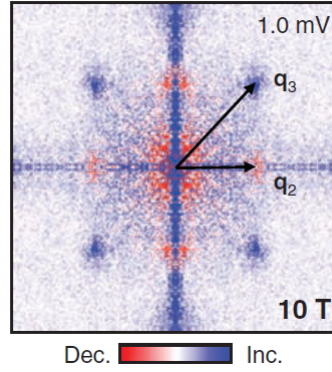


Figure 1.8: Effect of magnetic field in QPI intensities. This image is a result of subtracting the images obtained by FT of the STM image at 10 T and at 0 T. We can clearly distinguish an enhancing of the q_3 intensity and a suppression of the q_2 intensity as expected for an $s_{\pm}$ pairing symmetry. From [4]. Reprinted with permission from AAAS.

scattering through a magnetic field. Vortices act as magnetic sources of scattering enhancing sign preserving processes and suppressing sign changing processes [50]. Hanaguri *et al.* measured an enhancement in the QPI intensity for the scattering vector q_3 and a suppression for the scattering vector q_2 induced by magnetic field in Fe(Te,Se) [4]. The effect of magnetic field in the QPI intensities is shown in Figure 1.8. These results give strong evidence for the proposed $s_{\pm}$ -wave order parameter.

To obtain a definite determination of the order parameter of iron based superconductors more experiments are needed. STM measurements may be difficult to perform, due to experimental difficulties, such as the inability to grow a large enough sample, or may not reflect the bulk properties of the material. The iron based superconductor families better suited for STM analysis are the 11 and 111 families [51]. Besides Hanaguri *et al.*'s experiment, only another QPI measurement on LiFeAs has been reported [52]. According to calculations of the authors, the results of this experiment are not consistent with either s , $s_{\pm}$, or d -wave symmetry. They claim that the best match is p -wave symmetry but they also suggest a more exotic symmetry, such as $s + id$. Still, it has been claimed their STM images were not consistent with other STM measurements performed on LiFeAs [51].

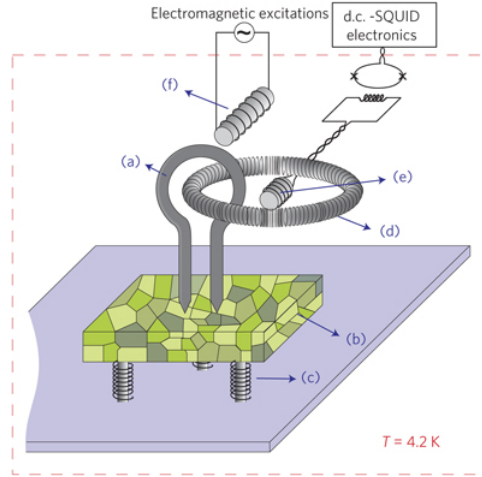


Figure 1.9: Experimental set-up used by Chen *et al.* . The composite loop is made of a Nb wire (a) pressed against the Nd-1111 sample (b) to form a complete circuit. The contact strength between the sample and the Nb tips is controlled by three Cu-Be spring-loaded brass screws (c). The Nb toroidal coil (d) applies magnetic flux to the loop from a low-noise current source by means of a twisted pair of leads. The Nb pickup coil (e) couples the induced flux to a commercial d.c.-SQUID as a magnetometer to monitor the flux states of the loop. The Nb solenoid (f) coupled to the composite loop transmits electromagnetic pulses from the external world to induce transitions between different quantized flux states. Reprinted by permission from Macmillan Publishers Ltd: [Nature] [1], copyright (2010).

1.6 Half integer and integer flux quantum transitions in a Nb-NdFeAsO_{0.88}F_{0.12} composite loop

Using the experimental setup shown in Figure 1.9, Chen *et al.* measured both integer and half-integer flux quantum transitions in a composite loop made of Niobium and NdFeAsO_{0.88}F_{0.12}. They were able to obtain these two types of flux quantum transitions by exciting the loop with electromagnetic pulses and measuring how the flux inside the loop relaxes as a function of time after the pulse has passed. The frequency of the integer flux quantum transitions was measured to be much higher than that of the half quantum transitions. Also, the frequency of half integer flux quantum transitions was measured to rise by increasing the critical current of the junction, which was done by increasing the strength of the contact between the two superconductors [1].

This experiment provides strong evidence for an unconventional order parameter. However, the results are surprising since neither conventional or π shifted Josephson junctions allow for the possibility of half-integer flux quantum transitions. It has been shown that within a modified Ginzburg-Landau model the results of the experiment can be explained by an unusual energy dependence on the flux quantum [53]. In this model, an order parameter with $s_{\pm}$ symmetry allows for three types of energy-flux relation: 1) a “time reversal symmetry breaking” regime where the energy has maxima at half integer and integer flux quantum values, and minima at some intermediate value; 2) a “single minimum” regime where the energy has minima at integer flux quantum values; and 3) a “double minimum” regime in which the energy has minima at half integer and integer flux quantum values. In the third regime, the minima at integer flux quantum values are global while the minima at half integer flux quantum are local. Accordingly, the experiment can be explained by arguing that the Nb-NdFeAsO_{0.88}F_{0.12} composite loop falls in the third regime. Through the electromagnetic excitations, the system is forced to switch between local-energy-minimum configurations, these result in half integer and integer flux quantum transitions. Since the integer flux quantum configurations are global energy minima then much more integer flux quantum transitions are observed.

Inspired by these results, this thesis will consist of finding the energy dependence on the flux in the loop for a composite loop formed by two junctions between an s -wave and an iron-pnictide superconductor within a microscopic model. We are specially interested in finding an energy-flux relation with minima at half integer and integer flux quantum values. While the Ginzburg-Landau model is suggestive, it is still phenomenological at best. We believe that a microscopic model could provide a solid framework and strengthen the claim that the experiment indeed supports the $s_{\pm}$ scenario. It also would be useful to find which microscopic conditions result in each of the three regimes obtained for the Ginzburg-Landau model. This may help to predict the behaviour of different compounds.

1.7 Summary and Thesis structure

Iron based superconductors are very intriguing materials. They seem to harbour an unconventional pairing mechanism, and to provide a new way to reach high temperature superconductivity, which makes important to study them for both practical and fundamental reasons. Furthermore, the complex band structure of these compounds, their Fermi surface structure and the intricate nature of the magnetic interactions in them, make the physics in them very rich and captivating. Determining the pairing symmetry in this family of superconductors is a key step to answer the more fundamental question of what is the mechanism that drives the Cooper pairing in these compounds. Most current theories favour an unconventional pairing mechanism and an $s_{\pm}$ pairing symmetry. Yet due to the lack of phase sensitive experiments capable of distinguishing between this type of symmetry and a conventional s -wave symmetry, this supposition remains unconfirmed.

Although there are many theoretical proposals, only two phase sensitive experiments whose results seem to provide evidence for the much predicted $s_{\pm}$ pairing structure have been performed. The first one is the experiment done by Chen *et al.* [1], described in the previous section. The second one, performed by Hanaguri *et al.*, uses STM to measure the quasi-particle interference spectrum. Chen *et al.*'s experiment has the advantage that it can be done in more compounds of the iron based superconducting family, contrary to the STM measurements that require the growth of large enough samples. This experiment and the modified Ginzburg-Landau model proposed to explain it [53] are the main inspiration for this work. The objective of this thesis is to present a microscopic model to study a magnetic flux threaded iron pnictide/ s -wave superconductor composite loop. We believe that this could provide a better understanding of the experiment results. It would also give more strength to the claim that these results are in agreement with the predicted $s_{\pm}$ symmetry.

We have organized this thesis in five chapters, the first one is this introduction. In the

second chapter, we will study the effects of magnetic flux in an s -wave superconductor loop. In the third chapter, we will analyse a flux threaded iron-pnictide superconductor loop. These two chapters will serve us to analyse the effects of magnetic flux on a simple setting and to introduce the models that we will use to treat both types of superconductors. In the fourth chapter, we will present the model for the magnetic flux threaded iron pnictide/ s -wave superconductor composite loop together with some preliminary results. Finally, we will state our conclusions in the last chapter.

***s*-wave loop**

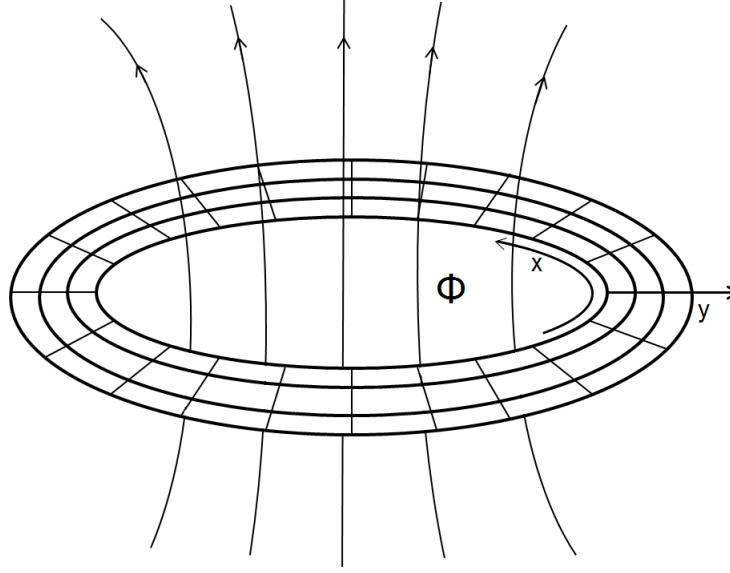
In this work, we are interested in obtaining the energy-flux relation for a composite loop formed by an *s*-wave and an $s_{\pm}$ superconductor. As a warm-up, we will start by studying the more simple problem of a flux threaded *s*-wave superconducting loop. This will allow us to see how magnetic flux influences a superconductor in a simple setting. Additionally, we will start developing the formalism needed to treat the composite loop.

To model the *s*-wave superconductor loop, we will consider a square lattice with one orbital per site, N_x sites on the x -direction and N_y sites on the y -direction (giving a total number of sites $N = N_x N_y$), with periodic boundary conditions. We will use a negative U-Hubbard Hamiltonian with nearest-neighbour hopping with an amplitude t , since it is the simplest possible model that results in *s*-wave superconductivity. We proceed to write our Hamiltonian,

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} c_{\sigma}^{\dagger}(\mathbf{r}) c_{\sigma}(\mathbf{r}') + U \sum_{\mathbf{r}} c_{\uparrow}^{\dagger}(\mathbf{r}) c_{\downarrow}^{\dagger}(\mathbf{r}) c_{\downarrow}(\mathbf{r}) c_{\uparrow}(\mathbf{r}) - \mu \sum_{\mathbf{r}, \sigma} c_{\sigma}^{\dagger}(\mathbf{r}) c_{\sigma}(\mathbf{r}) \quad (2.0.1)$$

where the operator $c_{\sigma}(\mathbf{r})$ annihilates an electron in site $\mathbf{r}$, μ is the chemical potential, and $U < 0$.

The periodic boundary conditions imply that $c_{\sigma}(\mathbf{r}) = c_{\sigma}(\mathbf{r} + aN_x \hat{x}) = c_{\sigma}(\mathbf{r} + aN_y \hat{y})$,

Figure 2.1: Superconductor loop subjected to a magnetic flux Φ .

where a is the lattice constant. For simplicity we will set the lattice constant to 1. Since the problem has discrete translational invariance, it will be useful to introduce the momentum space operators $c_{\mathbf{k},\sigma}$, which are given by:

$$c_{\sigma}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (2.0.2)$$

In terms of the operators $c_{\mathbf{k},\sigma}$, the Hamiltonian in equation (2.0.1) becomes:

$$H = \sum_{\mathbf{k},\sigma} (-2t \cos(k_x) - 2t \cos(k_y) - \mu) c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \frac{U}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k}+\mathbf{q},\downarrow}^{\dagger} c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}',\uparrow} \quad (2.0.3)$$

2.1 Magnetic flux

Now that we have written the Hamiltonian for our s -wave superconductor, we proceed to add the effect of the magnetic flux. We consider the arrangement shown in Figure 2.1, which consists of an s -wave superconductor ring with N_x lattice sites in the angular direction, N_y lattice sites in the radial direction, and a magnetic flux Φ penetrating the area

enclosed by the ring. We can select a gauge so that the magnetic potential is parallel to the angular direction, i.e. $\mathbf{A} = A\mathbf{e}_\theta$. Since we must have $\Phi = \oint \mathbf{A} \cdot d\mathbf{l}$, the vector potential in this gauge is equal $\mathbf{A} = \frac{\Phi}{2\pi r}\mathbf{e}_\theta$. The introduction of a magnetic potential in a tight binding model can be taken into account through the Peierls substitution.

$$H = - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} t(\mathbf{r}, \mathbf{r}') c_\sigma^\dagger(\mathbf{r}) c_\sigma(\mathbf{r}') + U \sum_{\mathbf{r}} c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) - \mu \sum_{\mathbf{r}, \sigma} c_\sigma^\dagger(\mathbf{r}) c_\sigma(\mathbf{r}) \quad (2.1.1)$$

$$t(\mathbf{r}, \mathbf{r}') = t \exp \left(-\frac{ie}{\hbar c} \int_{\mathbf{r}'}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{l} \right) \quad (2.1.2)$$

If we have N_x lattice sites in a circle of radius r , then $2\pi r = N_x$, where r is measured in units of the lattice constant. Therefore, the phase acquired by hopping from lattice site $m+1$ to lattice site m is:

$$\phi(\Phi) = -\frac{e}{\hbar c} \int_{\mathbf{r}'}^{\mathbf{r}} \mathbf{A} \cdot d\mathbf{l} = \frac{e\Phi a}{\hbar c 2\pi r} = \frac{e\Phi}{\hbar c N_x} = \frac{\pi}{N_x} \left(\frac{\Phi}{\Phi_0} \right) \quad (2.1.3)$$

with $\Phi_0 = \frac{hc}{2e}$ the superconducting flux quantum.

We now can write the Hamiltonian of the system for all values of the magnetic flux.

$$\begin{aligned} H(\Phi) = & \sum_{m,n,\sigma} \left(-te^{-i\phi(\Phi)} c_\sigma^\dagger(m+1, n) c_\sigma(m, n) - te^{i\phi(\Phi)} c_\sigma^\dagger(m, n) c_\sigma(m+1, n) \right. \\ & \left. - tc_\sigma^\dagger(m, n+1) c_\sigma(m, n) - tc_\sigma^\dagger(m, n) c_\sigma(m, n+1) - \mu c_\sigma^\dagger(m, n) c_\sigma(m, n) \right) \\ & + U \sum_{m,n} c_\uparrow^\dagger(m, n) c_\downarrow^\dagger(m, n) c_\downarrow(m, n) c_\uparrow(m, n) \end{aligned} \quad (2.1.4)$$

As it is evident in equation (2.1.3), the Peierls phase acquired from hopping from a site $m+1$ to a site m does not depend on m . This means that the kinetic part of the above

Hamiltonian can be decoupled in momentum space.

$$\begin{aligned}
 H(\Phi) = & \sum_{\mathbf{k},\sigma} (-2t \cos(k_x - \phi(\Phi)) - 2t \cos(k_y) - \mu) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \\
 & + \frac{U}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q},\downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}',\uparrow}
 \end{aligned} \tag{2.1.5}$$

Hence, the effect of the magnetic flux in the superconducting loop is to shift the Brillouin zone by a flux dependant phase $\phi(\Phi)$.

2.2 Mean-field solution

The interaction term in equation (2.1.5) can be decoupled using self-consistent mean-field theory, resulting in the mean-field Hamiltonian:

$$\begin{aligned}
 H(\Phi) \approx & \sum_{\mathbf{k},\sigma} (-2t \cos(k_x - \phi(\Phi)) - 2t \cos(k_y) - \mu) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \\
 & + \sum_{\mathbf{k},\mathbf{q}} \left(\Delta(\mathbf{q}) c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q},\downarrow}^\dagger + \Delta(\mathbf{q})^* c_{-\mathbf{k}+\mathbf{q},\downarrow} c_{\mathbf{k},\uparrow} \right) - \frac{N}{U} \sum_{\mathbf{q}} |\Delta(\mathbf{q})|^2
 \end{aligned} \tag{2.2.1}$$

and the self-consistent equations,

$$\Delta(\mathbf{q}) = \frac{U}{N} \sum_{\mathbf{k}} \langle c_{-\mathbf{k}+\mathbf{q},\downarrow} c_{\mathbf{k},\uparrow} \rangle \tag{2.2.2}$$

We can relate $\mathbf{q}$ to the center of mass momentum of the Cooper pairs. In the absence of magnetic flux, the ground state of the system is given by a condensate whose center of mass momentum is equal to zero, i.e. $\Delta(\mathbf{q}) = \delta(\mathbf{q})\Delta_0$. However, the effect of the magnetic flux in the loop can result in a moving condensate, i.e. supercurrent. Due to the symmetry of the problem, we still expect to have the same pair momentum for all Cooper pairs. Also, since the magnetic flux only shifts the Brillouin zone in the x -direction, the y -component of

the Cooper pair momentum should be equal to zero in the ground state. Therefore, we will solve the self-consistency equations by using an ansatz of the form $\Delta(\mathbf{q}') = \delta(\mathbf{q}' - \mathbf{q})\Delta_{\mathbf{q}}$ for all values of $\mathbf{q}$, such that $\mathbf{q} = \frac{2\pi n}{N_x}\hat{x}$, with $n = 0, 1, \dots, N_x - 1$. We can then pick the ground state of the system by choosing the value of $\mathbf{q}$ that minimizes the energy for each given value of the magnetic flux.

To solve the self-consistency equations (2.2.2), we need to diagonalize the mean-field Hamiltonian via a Bogoliubov transformation. We can rewrite the Hamiltonian for a given value of the Cooper pairs momentum in the following matrix form:

$$H_{\mathbf{q}}(\phi) = \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k},\uparrow}^\dagger & c_{-\mathbf{k}+\mathbf{q},\downarrow} \end{pmatrix} \begin{pmatrix} \xi(\mathbf{k}, \phi) & \Delta_{\mathbf{q}}^*(\phi) \\ \Delta_{\mathbf{q}}(\phi) & -\xi(-\mathbf{k} + \mathbf{q}, \phi) \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{-\mathbf{k}+\mathbf{q},\downarrow}^\dagger \end{pmatrix} - \frac{N}{U} |\Delta_{\mathbf{q}}(\phi)|^2 - \mu N \quad (2.2.3)$$

In this equation, we have denoted $\xi(\mathbf{k}, \phi) = -2t \cos(k_x - \phi) - 2t \cos(k_y) - \mu$. Besides, since the magnetic flux only enters the Hamiltonian through the phase $\phi(\Phi)$ given by equation (2.1.3), we have dropped the dependence on Φ to simplify the notation. Likewise, since the term $-\mu N$ is a flux independent constant, we will drop it in future calculations. We can now proceed to diagonalize the Hamiltonian using a set of unitary transformations $U_{\mathbf{q}}(\mathbf{k}, \phi)$, which fulfil the following equations.

$$\begin{pmatrix} \xi(\mathbf{k}, \phi) & \Delta_{\mathbf{q}}^*(\phi) \\ \Delta_{\mathbf{q}}(\phi) & -\xi(-\mathbf{k} + \mathbf{q}, \phi) \end{pmatrix} = U_{\mathbf{q}}(\mathbf{k}, \phi) \begin{pmatrix} E_{\mathbf{q},+}(\mathbf{k}, \phi) & 0 \\ 0 & E_{\mathbf{q},-}(\mathbf{k}, \phi) \end{pmatrix} U_{\mathbf{q}}(\mathbf{k}, \phi)^\dagger \quad (2.2.4)$$

Since $U_{\mathbf{q}}(\mathbf{k}, \phi)$ is a two-dimensional unitary matrix, it can be written as:

$$U_{\mathbf{q}}(\mathbf{k}, \phi) = \begin{pmatrix} u_{\mathbf{q}}(\mathbf{k}, \phi) & v_{\mathbf{q}}(\mathbf{k}, \phi) \\ -v_{\mathbf{q}}(\mathbf{k}, \phi)^* & u_{\mathbf{q}}(\mathbf{k}, \phi)^* \end{pmatrix} \quad (2.2.5)$$

The eigenvalues, $E_{\mathbf{q},\pm}(\mathbf{k}, \phi)$, and the Bogoliubov factors, $u_{\mathbf{q}}(\mathbf{k}, \phi)$ and $v_{\mathbf{q}}(\mathbf{k}, \phi)$, defined

by the equations (2.2.4) and (2.2.5) are given by:

$$\begin{aligned}
E_{\mathbf{q},\pm}(\mathbf{k}, \phi) &= \frac{\xi(\mathbf{k}, \phi) - \xi(-\mathbf{k} + \mathbf{q}, \phi)}{2} \pm \sqrt{|\Delta_{\mathbf{q}}(\phi)|^2 + \left(\frac{\xi(\mathbf{k}, \phi) + \xi(-\mathbf{k} + \mathbf{q}, \phi)}{2} \right)^2} \\
|u_{\mathbf{q}}(\mathbf{k}, \phi)|^2 &= \frac{E_{\mathbf{q},+}(\mathbf{k}, \phi) + \xi(-\mathbf{k} + \mathbf{q}, \phi)}{E_{\mathbf{q},+}(\mathbf{k}, \phi) - E_{\mathbf{q},-}(\mathbf{k}, \phi)} \\
|v_{\mathbf{q}}(\mathbf{k}, \phi)|^2 &= \frac{E_{\mathbf{q},+}(\mathbf{k}, \phi) - \xi(\mathbf{k}, \phi)}{E_{\mathbf{q},+}(\mathbf{k}, \phi) - E_{\mathbf{q},-}(\mathbf{k}, \phi)} \\
\arg \left(\frac{v_{\mathbf{q}}(\mathbf{k}, \phi)}{u_{\mathbf{q}}(\mathbf{k}, \phi)} \right) &= \arg (\Delta_{\mathbf{q}}(\phi))
\end{aligned} \tag{2.2.6}$$

We can see that for $\mathbf{q} = 0$ and $\phi = 0$, this set of equations yields the eigenvalues and Bogoliubov factors given by BCS theory.

We now proceed to write the self-consistency equation in terms of the Bogoliubov factors and the eigenenergies. This gives:

$$\Delta_{\mathbf{q}}(\phi) = \frac{U}{N} \sum_{\mathbf{k}} u_{\mathbf{q}}(\mathbf{k}, \phi)^* v_{\mathbf{k}}(\mathbf{q}, \phi) (f(E_{\mathbf{q},+}(\mathbf{k}, \phi)) - f(E_{\mathbf{q},-}(\mathbf{k}, \phi))) \tag{2.2.7}$$

where $f(E)$ is the Fermi-Dirac distribution. For simplicity, we will be working at zero temperature. The Fermi-Dirac distribution for $T = 0$ is $f(E) = 1 - \Theta(E)$, and, therefore, the self-consistency equation reduces to:

$$\Delta_{\mathbf{q}}(\phi) = -\frac{U}{N} \sum_{\mathbf{k}} u_{\mathbf{q}}(\mathbf{k}, \phi)^* v_{\mathbf{q}}(\mathbf{k}, \phi) \tag{2.2.8}$$

For any given value of the magnetic flux Φ , we can solve the self-consistency equation for each of the possible values of the Cooper pairs center of mass momentum $\mathbf{q}$ and then choose the ground state from the solution that minimizes the energy. In order to do this, we need to write the energy in terms of the eigenenergies of the system and the Bogoliubov

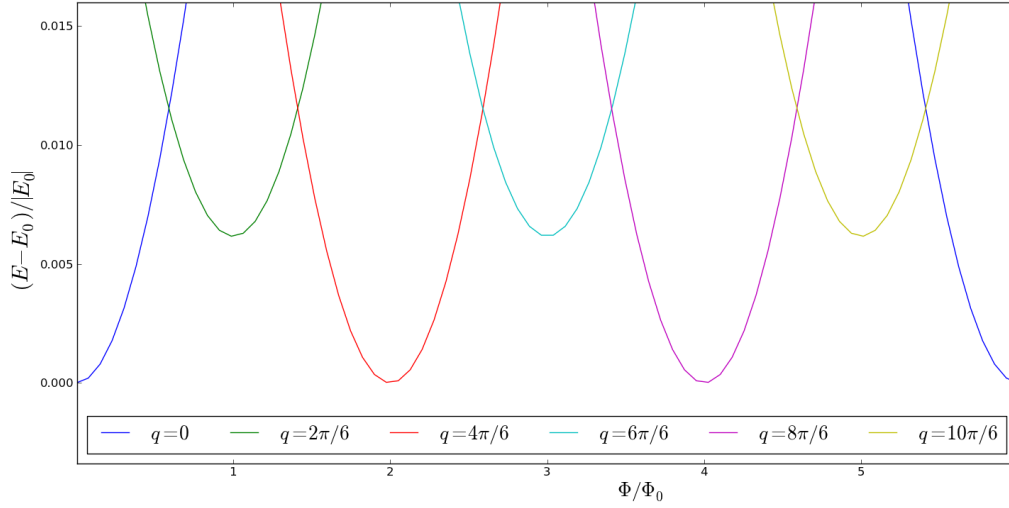


Figure 2.2: Energy dependence on flux for the possible values of q_x and the choice of parameters $t = 1$, $U = -3$, $\mu = 1.8$, $N_x = 6$, $N_y = 4$ at zero temperature. E_0 corresponds to the ground state energy of the system for $\Phi = 0$.

factors, which yields:

$$\begin{aligned}
 E_{\mathbf{q}}(\phi) &= \langle H(\phi) \rangle \\
 &= \sum_{\mathbf{k}} (E_{\mathbf{q},+}(\mathbf{k}, \phi) f(E_{\mathbf{q},+}(\mathbf{k}, \phi)) + E_{\mathbf{q},-}(\mathbf{k}, \phi) f(E_{\mathbf{q},-}(\mathbf{k}, \phi)) - \frac{N}{U} |\Delta_{\mathbf{q}}(\phi)|^2) \\
 &= \sum_{\mathbf{k}} E_{\mathbf{q},-}(\mathbf{k}, \phi) - \frac{N}{U} |\Delta_{\mathbf{q}}(\phi)|^2
 \end{aligned} \tag{2.2.9}$$

We can find a solution to the self-consistency equation (2.2.8) numerically for each value of $\mathbf{q}$ using an iterative method. In Figure 2.2, we can see that when we increase the magnetic flux inside the loop it becomes more energetically convenient for the condensate of pairs to increase its center of mass momentum. The minima of the energy are as expected in integer multiples of the superconducting flux quantum, nonetheless, the energy at even multiples is lower than the one at odd multiples. This is an artefact of the finite size system, and in the thermodynamic limit the periodicity of the energy becomes Φ_0 . We can notice this in Figure 2.3, where by increasing the size of the lattice we have made the difference

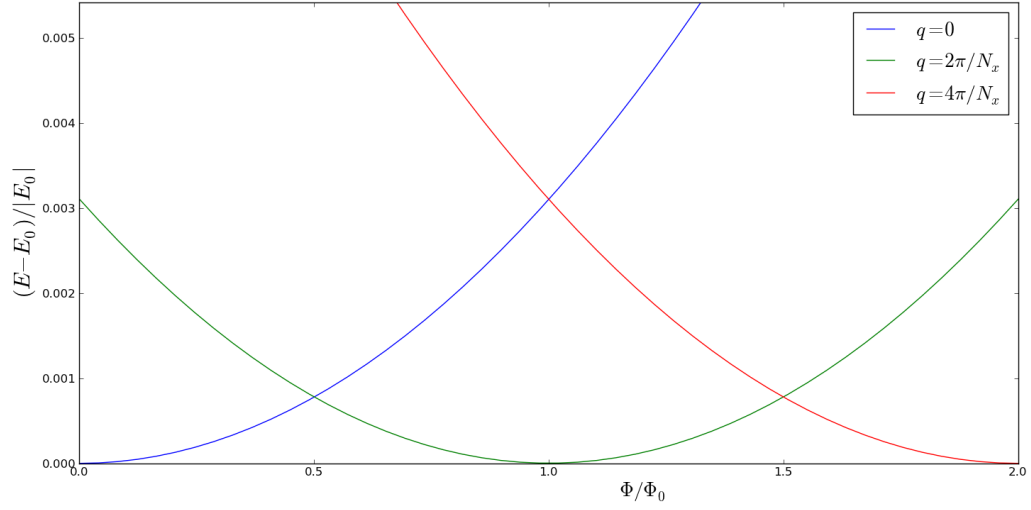


Figure 2.3: Energy dependence on flux for $t = 1$, $U = -3$, $\mu = 1.8$, $N_x = 20$, $N_y = 10$ at zero temperature.

between the minimum at $\Phi = 0$ and the one at $\Phi = \Phi_0$ practically indistinguishable.

2.3 Discussion

The energy-flux relations shown in Figure 2.2 and Figure 2.3 are in agreement with [54]. The difference in the energy for odd integers and even integers flux quantum values visible in Figure 2.2 is caused by the difference of eigenenergies between the $\mathbf{k}$ values in the phase shifted Brillouin zone and the $\mathbf{k}$ values in the normal Brillouin zone. In the thermodynamic limit, the allowed values of $\mathbf{k}$ become continuous, this closes the energy difference between odd integers and even integers flux quantum values, and changes the periodicity of the flux-energy relation. This change of periodicity is a signature of the superconducting state, as opposed to the normal state where quantities are periodic in flux with a normal flux quantum hc/e period.

In the previous section, we solved the self-consistency equations by assuming a state where all the Cooper pairs have the same center of mass momentum. This ensures the gauge

invariance of the Hamiltonian, and allows us to find the ground state solution. However, one may ask if a solution with different pairing momenta is allowed. For the model presented in this chapter, all the solutions of equation (2.2.2) are indeed of the form $\Delta(\mathbf{q}') = \delta(\mathbf{q}' - \mathbf{q})\Delta_{\mathbf{q}}$. This is the case for all *s*-wave superconductors.

Be that as it may, for superconductors with unconventional symmetry, it may be possible to find a solution where not all the Cooper pairs have the same momentum. An example of this type of solution is the “pair density wave” (PDW) state, which consists of a state in which Cooper pairs with momentum $\mathbf{q}$ and $-\mathbf{q}$ coexist. The PDW state has been shown to be a possible solution for *d*-wave superconductivity [55] [56], and it has been proposed to account for experimental anomalies observed in some high T_c cuprate superconductors, such as, $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ [55].

Finally, it is useful to look at the real space dependence of the order parameter of the *s*-wave loop. Mean-field decoupling the interaction term in real space results in the term $\sum_{\mathbf{r}} \left(\Delta(\mathbf{r})c_{\uparrow}^{\dagger}(\mathbf{r})c_{\downarrow}^{\dagger} + \Delta(\mathbf{r})^*c_{\downarrow}(\mathbf{r})c_{\uparrow}(\mathbf{r}) - \frac{|\Delta(\mathbf{r})|^2}{U} \right)$, with the real space order parameter $\Delta(\mathbf{r})$ defined as $\Delta(\mathbf{r}) = U \langle c_{\downarrow}(\mathbf{r})c_{\uparrow}(\mathbf{r}) \rangle$. A solution given by $\Delta(\mathbf{q}') = \delta(\mathbf{q}' - \mathbf{q})\Delta_{\mathbf{q}}$, where all the Cooper pairs have the same momentum, results in a real space order parameter of the form $\Delta(\mathbf{r}) = \Delta_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{r}}/N$.

Iron-pnictide loop

In this chapter, we will start by introducing the models we use to treat the band structure and the pairing mechanism of the iron based superconductor. For the band structure we will use a minimal two band model [57]; for the pairing mechanism, a nearest neighbours and next-nearest neighbours anti-ferromagnetic coupling [5]. We will show that for the correct choice of parameters this model results in superconductivity with $s_{\pm}$ symmetry, which is the superconducting structure favoured by most theories for the iron based superconductors. Afterwards, we will add flux to the loop following the arrangement shown in Figure 2.1, as in the previous chapter. The purpose of this chapter is to describe how we will model the iron-pnictide part of the composite loop in the next chapter, and to find out if the qualitative behaviour of an $s_{\pm}$ superconducting loop is in any way different from the one found in the previous chapter for an s -wave loop.

3.1 Minimal two band model

As it was mentioned in the introduction of this thesis, the superconducting electrons in iron based superconductors live in the corrugated layers formed by iron and a pnictogen (or chalcogen). This layer, shown in Figure 3.1, consist of Fe ions forming a square lattice,

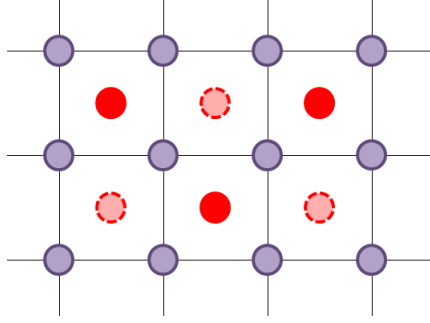


Figure 3.1: Scheme of the Fe layer. The Fe-ions are represented in purple, the above plane pnictogen ions are solid red and the below plane pnictogen ions are dashed.

and pnictogen (or chalcogen) ions located directly above or directly below the center of the squares formed by the Fe ions. The unit cell of this two-dimensional lattice includes two Fe ions and two pnictogen (or chalcogen) ions.

The main features of the rich electronic structure of the iron-pnictides are: 1) a fermi surface consisting of two quasi-cylindrical electron pockets located around the M point and two quasi-cylindrical hole pockets around the Γ point; and 2) a multi-band band structure that, close to the Fermi surface, is dominated by the five $3d$ orbitals of the Fe ions. This image gets further complicated by the fact that the dominant Fe- $3d$ orbitals hybridize among themselves and through the pnictogen orbitals.

In order to find a simple model that describes the iron-pnictide electronic structure it is better to only consider the square lattice formed by the Fe ions. In this description the unit cell is formed by only one Fe ions, as opposed to the crystallographic cell which consists of two Fe and two pnictogen ions. The Brillouin zone is twice the size of the original Brillouin zone and it is rotated 45° . It is easy to go from the one Fe ion unit cell description to the true crystallographic description by folding the Brillouin zone.

Out of the five $3d$ orbitals from the Fe ions, the greatest contribution close to the Fermi surface comes from the d_{xz} , d_{yz} and d_{xy} orbitals. The two hole pockets around Γ originate from the d_{xz} and the d_{yz} bands. Additionally, in the unfolded Brillouin zone the two electron pockets become one electron pocket originated by the d_{xz} and the d_{yz} bands hybridized

with the d_{xy} band [58]. Now that we have reduced the number of orbitals from five to three, we must also consider the overlap between Fe orbitals and the pnictogen orbitals. This leads to an effective pnictogen mediated NNN hopping between the Fe orbitals. Hence, any tight binding model describing the iron-pnictides must include both NN and NNN hopping.

In this thesis we will use the minimal two band model proposed by Raghu *et al.* [57]. They make the further approximation that the d_{xy} orbital can be replaced by a NN hybridization between the d_{xz} and the d_{yz} orbitals. The model consists of a two dimensional square lattice with two orbitals per site (d_{xz} and d_{yz}) and four hopping parameters. First, we have a NN hopping t_1 for the direction in which the orbitals overlap end-to-end, i.e. hopping in the x -direction from a d_{xz} to a similar orbital, or hopping in the y -direction from a d_{yz} orbital to a d_{yz} orbital. The second hopping parameter t_2 is for NN hopping between orbitals that overlap side to side, this means hopping from a d_{yz} orbital to a d_{yz} orbital in the x -direction or hopping from a d_{xz} orbital to a d_{xz} orbital in the y -direction. We also have two NNN hopping parameters, t_3 between similar orbitals, and t_4 between different orbitals. The Hamiltonian for this model can be written as follows:

$$H_0 = \sum_{\mathbf{k}, \sigma} \Psi_{\mathbf{k}, \sigma}^\dagger \begin{pmatrix} \epsilon_x(\mathbf{k}) & \epsilon_{xy}(\mathbf{k}) \\ \epsilon_{xy}(\mathbf{k}) & \epsilon_y(\mathbf{k}) \end{pmatrix} \Psi_{\mathbf{k}, \sigma} \quad (3.1.1)$$

where $\Psi_{\mathbf{k}, \sigma}^\dagger = (d_{x, \mathbf{k}, \sigma}^\dagger, d_{y, \mathbf{k}, \sigma}^\dagger)$, the operators $d_{x, \mathbf{k}, \sigma}^\dagger$ and $d_{y, \mathbf{k}, \sigma}^\dagger$ create an electron with momentum $\mathbf{k}$ and spin σ on the $3d_{xz}$ orbital and on the $3d_{yz}$ orbital, respectively, and,

$$\begin{aligned} \epsilon_x(\mathbf{k}) &= -2t_1 \cos(k_x) - 2t_2 \cos(k_y) - 4t_3 \cos(k_x) \cos(k_y) - \mu \\ \epsilon_y(\mathbf{k}) &= -2t_2 \cos(k_x) - 2t_1 \cos(k_y) - 4t_3 \cos(k_x) \cos(k_y) - \mu \\ \epsilon_{xy}(\mathbf{k}) &= -4t_4 \sin(k_x) \sin(k_y) \end{aligned} \quad (3.1.2)$$

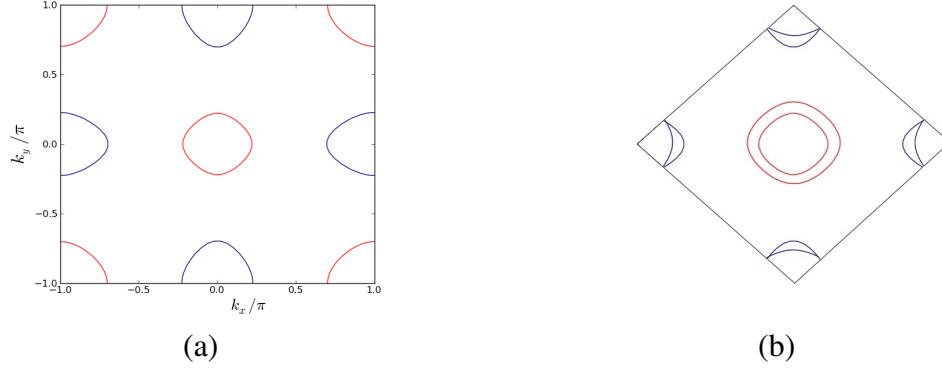


Figure 3.2: (a) Fermi surface of the minimal two band model for the specific choice of parameters $t_1 = -1$, $t_2 = 1.3$, $t_3 = t_4 = -0.85$, at half filling ($\mu = 1.54$) in the unfolded Brillouin zone centred at the Γ point. The electron pockets are shown in blue and the hole pockets in red, folding this Fermi surface results in (b).

Diagonalizing this Hamiltonian leads to two energy bands given by:

$$E_{\pm}(\mathbf{k}) = \frac{1}{2} \left(\epsilon_x(\mathbf{k}) + \epsilon_y(\mathbf{k}) \pm \sqrt{(\epsilon_x(\mathbf{k}) - \epsilon_y(\mathbf{k}))^2 + \epsilon_{xy}(\mathbf{k})^2} \right) - \mu \quad (3.1.3)$$

The Fermi surface for the specific choice of parameters $t_1 = -1$, $t_2 = 1.3$, $t_3 = t_4 = -0.85$, at half-filling is shown in Figure 3.2. For this choice of parameters half-filling corresponds to $\mu = 1.54$. The Fermi surface in the folded Brillouin zone consists of two hole pockets (given by $E_- = 0$) and two electron pockets (given by $E_+ = 0$). Hence, using these parameters the Fermi surface for the minimal two band model has the same topology as the Fermi surface obtained by first principles band calculations and confirmed by ARPES measurements. Nonetheless, to obtain the correct relative size and the correct shape of the pockets it may be necessary to add, at least, a third orbital.

Raghu *et al.* also calculated the density of states (DOS) and the spin susceptibility for the above choice of parameters [57]. The DOS displays van Hove singularities, and the spin susceptibility shows a transition to an anti-ferromagnetic phase. Both of these results are in agreement with experimental and theoretical results on the iron-pnictide electronic structure. Therefore, we believe that the qualitative behaviour of the iron-pnictide band

structure can be obtained from this model. To get a full description of the low energy physics of the pnictides, it is necessary to consider the five $3d$ orbitals of the Fe ions. However, working with a five orbital description would make calculations lengthy and yield results far more difficult to interpret. The minimal two band model is the simplest possible model with a similar electronic structure to the ones obtained by first principles calculations, and it captures the fundamental physics of the iron-pnictides band structure.

3.2 Antiferromagnetic pairing

According to the current experimental and theoretical evidence, spin fluctuations are the most likely candidate for the pairing mechanism of the iron based superconductors. The complex magnetic structure of iron based compounds is mainly caused by three factors: 1) the proximity to a Stoner instability; 2) the SDW nesting between electron and hole pockets; and 3) the antiferromagnetic NN and NNN exchange. The structure of the antiferromagnetic phase in the iron-pnictide parent compounds can be obtained by an itinerant perturbative approach in the limit of weak interactions or in the limit of strong interactions by an antiferromagnetic $J_1 - J_2$ model with $2J_2 > J_1$. It should be noted that both limits fail to fully capture the physics of spin fluctuations in these materials.

Nevertheless, the superconducting structure obtained for both the weak and the strong correlations limit has the same symmetry: $s_{\pm}$. Since this thesis' concern is the experimental determination of the order parameter symmetry, we will leave the question of the correct description of magnetic interactions aside, and choose to particularize for one of the two solvable limits. We have chosen to use the antiferromagnetic coupling $J_1 - J_2$ model proposed by Seo *et al.* [5]. Although it is incompatible with the metallic nature of the iron based superconductors, we can obtain from this model the pairing symmetry we are interested in describing. The model is also simple, and it is consistent with the magnetic

structure of the iron based compounds.

The terms in the interaction Hamiltonian proposed by Seo *et al.* are: NN and NNN antiferromagnetic coupling between identical orbitals (intraband) and between different orbitals (interband); and Hund's rule coupling of spins of different orbitals on the same site. For simplicity, we will neglect the inter-orbital coupling and the Hund's rule coupling. Numerical results show that this decision does not affect the resulting pairing state symmetry [5]. With these simplifications, the resulting interaction Hamiltonian is given by:

$$\begin{aligned}
 V = - \sum_{\mathbf{r}, \alpha, i, \delta_i} J_i & \left(d_{\alpha, \uparrow}^\dagger(\mathbf{r}) d_{\alpha, \downarrow}^\dagger(\mathbf{r} + \delta_i) d_{\alpha, \downarrow}(\mathbf{r}) d_{\alpha, \uparrow}(\mathbf{r} + \delta_i) + d_{\alpha, \uparrow}^\dagger(\mathbf{r} + \delta_i) d_{\alpha, \downarrow}^\dagger(\mathbf{r}) d_{\alpha, \downarrow}(\mathbf{r} + \delta_i) d_{\alpha, \uparrow}(\mathbf{r}) \right. \\
 & \left. + d_{\alpha, \uparrow}^\dagger(\mathbf{r}) d_{\alpha, \downarrow}^\dagger(\mathbf{r} + \delta_i) d_{\alpha, \downarrow}(\mathbf{r} + \delta_i) d_{\alpha, \uparrow}(\mathbf{r}) + d_{\alpha, \uparrow}^\dagger(\mathbf{r} + \delta_i) d_{\alpha, \downarrow}^\dagger(\mathbf{r}) d_{\alpha, \downarrow}(\mathbf{r}) d_{\alpha, \uparrow}(\mathbf{r} + \delta_i) \right)
 \end{aligned} \quad (3.2.1)$$

In the above equation i takes the values of 1 and 2, 1 for NN coupling and 2 for NNN coupling. Hence $\delta_1 = \hat{x}, -\hat{x}, \hat{y}, -\hat{y}$, and $\delta_2 = \hat{x} + \hat{y}, -\hat{x} + \hat{y}, \hat{x} - \hat{y}, -\hat{x} - \hat{y}$. The index α indicates the orbital and takes the values of x and y , and both exchange constants are antiferromagnetic, i.e. $J_1, J_2 > 0$.

To take advantage of the translational invariance of the system, we will work in momentum space. The interaction term becomes:

$$V = \sum_{\alpha, \mathbf{k}', \mathbf{k}, \mathbf{q}} V(\mathbf{k}, \mathbf{k}', \mathbf{q}) d_{\alpha, \mathbf{k}, \uparrow}^\dagger d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow}^\dagger d_{\alpha, -\mathbf{k}' + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}', \uparrow} \quad (3.2.2)$$

$$\begin{aligned}
 V(\mathbf{k}, \mathbf{k}', \mathbf{q}) = & -\frac{2J_1}{N} \cos\left(k_x - \frac{q_x}{2}\right) \cos\left(k'_x - \frac{q'_x}{2}\right) - \frac{2J_1}{N} \cos\left(k_y - \frac{q_y}{2}\right) \cos\left(k'_y - \frac{q'_y}{2}\right) \\
 & - \frac{8J_2}{N} \cos\left(k_x - \frac{q_x}{2}\right) \cos\left(k_y - \frac{q_y}{2}\right) \cos\left(k'_x - \frac{q'_x}{2}\right) \cos\left(k'_y - \frac{q'_y}{2}\right) \\
 & - \frac{8J_2}{N} \sin\left(k_x - \frac{q_x}{2}\right) \sin\left(k_y - \frac{q_y}{2}\right) \sin\left(k'_x - \frac{q'_x}{2}\right) \sin\left(k'_y - \frac{q'_y}{2}\right)
 \end{aligned} \quad (3.2.3)$$

In the absence of magnetic flux, the ground state of the superconducting state will be

formed by Cooper pairs with zero center of mass momentum. From the form of $V(\mathbf{k}, \mathbf{k}', 0)$, it is evident that a mean field decoupling of the interaction will result in an order parameter where there is a mixture of four possible pairing symmetries: $s_{x^2+y^2} \sim \cos(k_x) + \cos(k_y)$ and $d_{x^2-y^2} \sim \cos(k_x) - \cos(k_y)$, which arise from the NN coupling, and $s_{x^2y^2} \sim \cos(k_x) \cos(k_y)$ and $d_{xy} \sim \sin(k_x) \sin(k_y)$, which come from the NNN coupling. Up to a constant, the effective mean field coupling is given by:

$$V_{MF} = \sum_{\mathbf{k}, \mathbf{k}', \alpha} \left(\Delta_{\alpha}(\mathbf{k}) d_{\alpha, \mathbf{k}, \uparrow}^{\dagger} d_{\alpha, -\mathbf{k}, \downarrow}^{\dagger} + \Delta_{\alpha}(\mathbf{k})^* d_{\alpha, -\mathbf{k}', \downarrow} d_{\alpha, \mathbf{k}', \uparrow} \right) \quad (3.2.4)$$

where the intra-orbital order parameter $\Delta_{\alpha}(\mathbf{k})$ can be written as $\Delta_{\alpha}(\mathbf{k}) = \Delta_{s_{x^2+y^2}, \alpha}(\cos(k_x) + \cos(k_y)) + \Delta_{d_{x^2-y^2}, \alpha}(\cos(k_x) - \cos(k_y)) + \Delta_{s_{x^2y^2}, \alpha} \cos(k_x) \cos(k_y) + \Delta_{d_{xy}, \alpha} \sin(k_x) \sin(k_y)$, and the amplitudes of the four different pairing symmetries are solutions to set of the self-consistency equations:

$$\begin{aligned} \Delta_{s_{x^2+y^2}, \alpha} &= -\frac{2J_1}{N} \sum_{\mathbf{k}} (\cos(k_x) + \cos(k_y)) \langle d_{\alpha, -\mathbf{k}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\ \Delta_{d_{x^2-y^2}, \alpha} &= -\frac{2J_1}{N} \sum_{\mathbf{k}} (\cos(k_x) - \cos(k_y)) \langle d_{\alpha, -\mathbf{k}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\ \Delta_{s_{x^2y^2}, \alpha} &= -\frac{8J_2}{N} \sum_{\mathbf{k}} \cos(k_x) \cos(k_y) \langle d_{\alpha, -\mathbf{k}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\ \Delta_{d_{xy}, \alpha} &= -\frac{8J_2}{N} \sum_{\mathbf{k}} \sin(k_x) \sin(k_y) \langle d_{\alpha, -\mathbf{k}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \end{aligned} \quad (3.2.5)$$

By solving the equations (3.2.5) near the critical temperature, i.e. $\Delta_{\alpha}(\mathbf{k}) \rightarrow 0$, Seo *et al.* found the phase diagram shown in Figure 3.3. The phase diagram consists in three phases: a phase on the upper corner with $s_{x^2y^2}$ symmetry, a phase in the down right corner with a mixture of $s_{x^2+y^2}$ and a small amount of $d_{x^2+y^2}$, and, finally, a phase where the order parameter is a mixture between $s_{x^2y^2}$ and a small amount of $d_{x^2-y^2}$. In the last phase, the pairing amplitudes $\Delta_{d_{x^2-y^2}, x}$ and $\Delta_{d_{x^2-y^2}, y}$ have opposite signs. For iron based supercon-

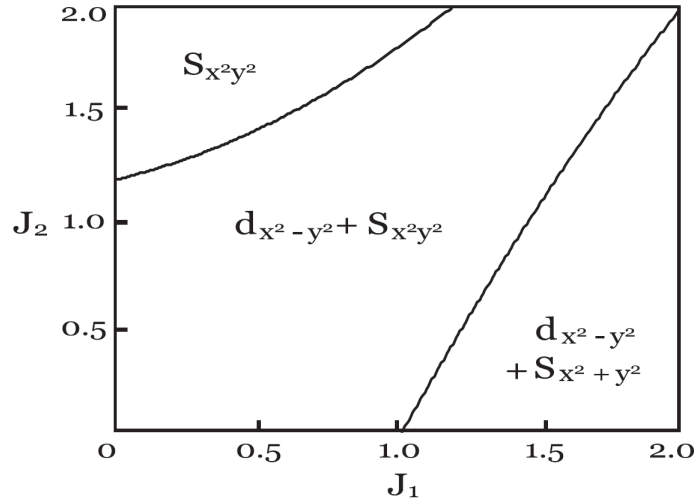


Figure 3.3: Phase diagram for $T \rightarrow T_c$ at 18% electron doping ($\mu = 1.8$). From [5]. Copyright (2008) by The American Physical Society.

ductors the strength between the two exchange constants, J_1 and J_2 , is comparable, and, according to calculations performed by references [24] and [28], $J_2 > J_1$. Therefore, the pairing symmetry predicted for the iron based superconductors from this model is $s_{x^2y^2}$.

The symmetry $s_{x^2y^2}$ corresponds to $s_{\pm}$ symmetry. In Figure 3.4 we can see that an order parameter of the form $\Delta_{\alpha}(\mathbf{k}) = \Delta_{s_{x^2y^2}} \cos(k_x) \cos(k_y)$ changes sign between the electron and hole pockets of the Fermi surface. For $J_2 > J_1$ it is easy to understand why the symmetry $s_{x^2y^2}$ dominates over the symmetries $s_{x^2+y^2}$ and $d_{x^2-y^2}$, since the former is caused by NNN exchange while the other two symmetries arise from the NN exchange. The reason why $s_{x^2y^2}$ symmetry dominates over d_{xy} symmetry is more subtle, and it is related to the structure of the Fermi surface. The peaks of the function $\cos(k_x) \cos(k_y)$ are exactly the points around which are the electron and hole pockets of the Fermi surface. On the other hand the peaks of the function $\sin(k_x) \sin(k_y)$ are at $(\pm\pi/2, \pm\pi/2)$. Since in superconductivity the pairing occurs around the Fermi surface, the dominant symmetry will be the one where the overlap between the symmetry factor ($\cos(k_x) \cos(k_y)$ or $\sin(k_x) \sin(k_y)$) and the Fermi surface is the largest. Another way to argue this dominance is to consider the

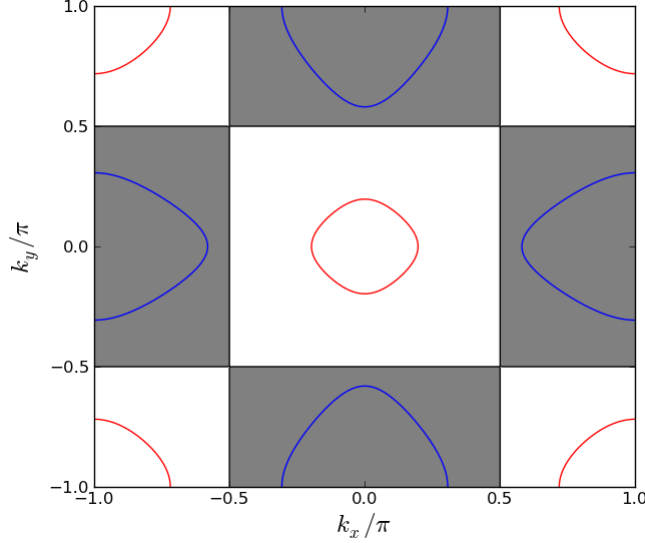


Figure 3.4: Fermi surface at 18% electron doping. The electron pockets are shown in blue and the hole pockets in red. The symmetry factor $\cos(k_x)\cos(k_y)$ corresponding to $s_{x^2y^2}$ symmetry is negative in the shaded areas and positive in the blank areas of the Brillouin zone.

overlap between the symmetry factor and the spectral function.

We can use the previous argument to say that the dominance of the $s_{x^2y^2}$ symmetry will be maintained if more orbitals are added to this model, as long as the structure of the Fermi surface, two electron pockets around the M point and two electron pockets around the Γ point, is kept. We would also like to mention that it is indispensable to have at least two orbitals to obtain this pairing symmetry. Models in the strong coupling limit considering only one orbital invariably predict a d_{xy} symmetry [24] [59] [60].

We solved the self-consistency equations numerically (3.2.5) at $T = 0$ for different values of J_1 and J_2 in a lattice of 40 sites in the x -direction and 40 sites in the y -direction. The procedure for solving the self-consistency equations is shown for a more general case in the next section. At $T = 0$, we find more mixture between the different pairing symmetries than in the phase diagram shown in Figure 3.3. The phase diagram for $T = 0$, shown in Figure 3.5, is a mixture of $s_{x^2y^2}$, $d_{x^2-y^2}$, and $s_{x^2+y^2}$. As for temperatures close to T_c , for $T = 0$ there is no d_{xy} contribution in the phase diagram. Even though there is more mixture

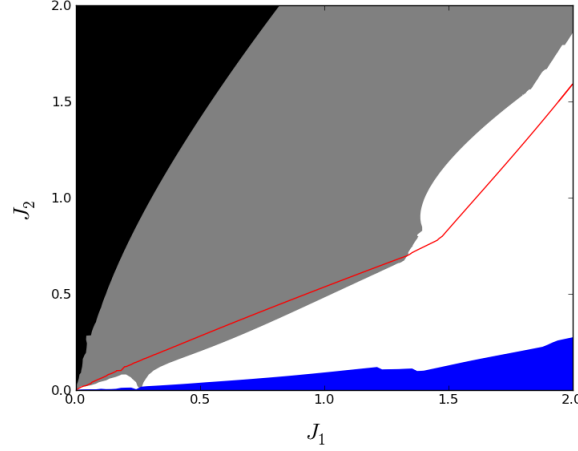


Figure 3.5: Phase diagram for $T = 0$ at 18% electron doping. In all the phase diagram, the order parameter is a mixture of $s_{x^2y^2}$, $d_{x^2-y^2}$, and $s_{x^2+y^2}$. The black area represents the parts of the phase diagram where the pairing amplitude for $s_{x^2y^2}$ symmetry is at least one order of magnitude larger than the pairing amplitudes for $d_{x^2-y^2}$ and $s_{x^2+y^2}$. In the gray area the symmetry is predominantly a mixture of $s_{x^2y^2}$ and $d_{x^2-y^2}$, with $s_{x^2+y^2}$ an order of magnitude smaller. In the blue area the pairing amplitudes for $d_{x^2-y^2}$ and $s_{x^2+y^2}$ are comparable, and the $s_{x^2y^2}$ pairing amplitude is an order of magnitude smaller. The three pairing amplitudes are comparable in the white area. The red line divides the phase diagram into two parts: 1) above the red line $s_{x^2y^2}$ is the predominant symmetry, i.e. the magnitude of the pairing amplitude $\Delta_{s_{x^2y^2}}$ is larger than the magnitude of any other pairing amplitude, and 2) below the red line $s_{x^2y^2}$ is no longer the predominant symmetry.

between the different pairing symmetries at $T = 0$, the overall pairing symmetry is $s_{\pm}$ for a considerable part of the phase diagram. Figure 3.6 displays the sign of the order parameter $\Delta_{\alpha}(\mathbf{k})$ for $J_1 = 0.5$ and $J_2 = 2.0$ at $T = 0$ and 18% electron doping. For this choice of parameters, the order parameter is $s_{x^2y^2}$ with a small mixture of $d_{x^2-y^2}$ and even smaller contribution of $s_{x^2+y^2}$. The pairing amplitudes $\Delta_{d_{x^2-y^2},x}$ and $\Delta_{d_{x^2-y^2},y}$ have opposite signs which leads to the difference observed between the two orbitals.

3.3 Flux threaded iron-pnictide loop

We now proceed to consider the effect of the magnetic flux in the model previously described. The addition of non-zero magnetic flux will have two effects in our Hamiltonian.

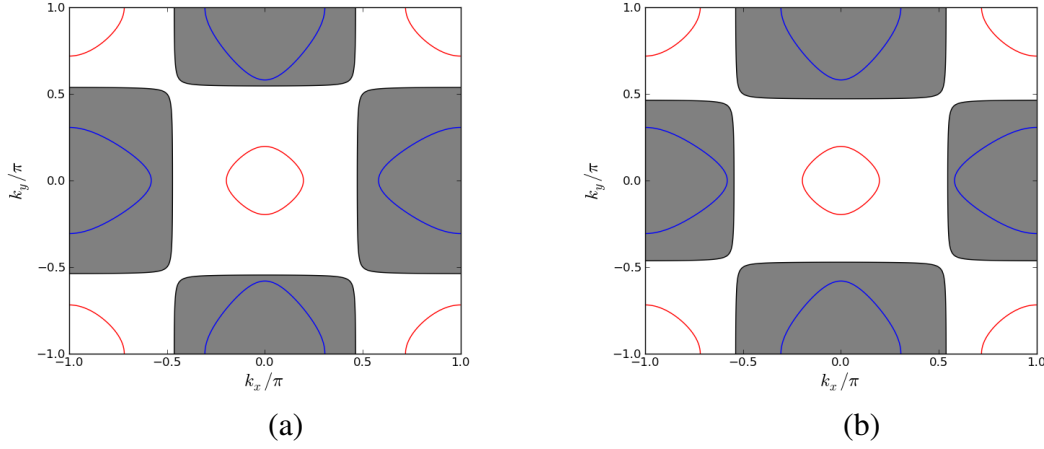


Figure 3.6: Sign of the order parameter $\Delta_\alpha(\mathbf{k})$ for $\alpha = x$ (a) and $\alpha = y$ (b) for $J_1 = 0.5$, $J_2 = 2.0$ at $T = 0$ and 18% electron doping. The shaded areas are the values of $\mathbf{k}$ for which the order parameter is negative. The Fermi surface is shown with the electron pockets in blue and the hole pockets in red.

First, the hopping terms in the kinetic part of the Hamiltonian will be transformed through Peierls substitution. Secondly, we can no longer assume that the condensate is static, so we must allow for the possibility of having a pairing momentum $\mathbf{q}$ different than zero. Hence, the Hamiltonian for the flux threaded loop in momentum space is:

$$\begin{aligned}
 H(\Phi) = & \sum_{\mathbf{k}, \sigma} \left(\epsilon_x(k_x - \phi(\Phi), k_y) d_{x, \mathbf{k}, \sigma}^\dagger d_{x, \mathbf{k}, \sigma} + \epsilon_y(k_x - \phi(\Phi), k_y) d_{y, \mathbf{k}, \sigma}^\dagger d_{y, \mathbf{k}, \sigma} \right. \\
 & + \epsilon_{xy}(k_x - \phi(\Phi), k_y) \left(d_{x, \mathbf{k}, \sigma}^\dagger d_{y, \mathbf{k}, \sigma} + d_{y, \mathbf{k}, \sigma}^\dagger d_{x, \mathbf{k}, \sigma} \right) \Big) \\
 & + \sum_{\alpha, \mathbf{k}', \mathbf{k}, \mathbf{q}} V(\mathbf{k}, \mathbf{k}', \mathbf{q}) d_{\alpha, \mathbf{k}, \uparrow}^\dagger d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow}^\dagger d_{\alpha, -\mathbf{k}' + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}', \uparrow}
 \end{aligned} \tag{3.3.1}$$

In the above Hamiltonian, $V(\mathbf{k}, \mathbf{k}', \mathbf{q})$ is given by equation (3.2.3), and the flux dependant Peierls phase by equation (2.1.3).

The next step is to use mean field theory to decouple the interaction term. Following the previous chapter, we will look for solutions in which all the Cooper pairs have the same momentum $\mathbf{q} = q\hat{x}$ with $q = \frac{2\pi n}{N_x}$ and $n = 0, 1, \dots, N_x - 1$. Afterwards, we will obtain the ground state of the system by selecting the value of $\mathbf{q}$ that minimizes the energy. The

mean-field Hamiltonian for a momentum pairing $\mathbf{q}$ is given by:

$$\begin{aligned}
 H_{\mathbf{q}}(\phi) = & \sum_{\mathbf{k}, \sigma} \left(\epsilon_x(k_x - \phi, k_y) d_{x, \mathbf{k}, \sigma}^\dagger d_{x, \mathbf{k}, \sigma} + \epsilon_y(k_x - \phi, k_y) d_{y, \mathbf{k}, \sigma}^\dagger d_{y, \mathbf{k}, \sigma} \right. \\
 & \left. + \epsilon_{xy}(k_x - \phi, k_y) \left(d_{x, \mathbf{k}, \sigma}^\dagger d_{y, \mathbf{k}, \sigma} + d_{y, \mathbf{k}, \sigma}^\dagger d_{x, \mathbf{k}, \sigma} \right) \right) \\
 & + \sum_{\alpha, \mathbf{k}} \left(\Delta_{\mathbf{q}, \alpha}(\mathbf{k}) d_{\alpha, \mathbf{k}, \uparrow}^\dagger d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow}^\dagger + \Delta_{\mathbf{q}, \alpha}(\mathbf{k})^* d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \right) + C_{\mathbf{q}}(\phi)
 \end{aligned} \tag{3.3.2}$$

The order parameter $\Delta_{\mathbf{q}, \alpha}(\mathbf{k})$ may be written as:

$$\begin{aligned}
 \Delta_{\mathbf{q}, \alpha}(\mathbf{k}) = & \Delta_{\mathbf{q}, s_{x^2+y^2}, \alpha} \left(\cos \left(k_x - \frac{q_x}{2} \right) + \cos(k_y) \right) + \Delta_{\mathbf{q}, d_{x^2-y^2}, \alpha} \left(\cos \left(k_x - \frac{q_x}{2} \right) - \cos(k_y) \right) \\
 & + \Delta_{\mathbf{q}, s_{x^2y^2}, \alpha} \cos \left(k_x - \frac{q_x}{2} \right) \cos(k_y) + \Delta_{\mathbf{q}, d_{xy}, \alpha} \sin \left(k_x - \frac{q_x}{2} \right) \sin(k_y)
 \end{aligned} \tag{3.3.3}$$

The pairing amplitudes, defined by the equation above, obey the next set of self-consistency equations:

$$\begin{aligned}
 \Delta_{\mathbf{q}, s_{x^2+y^2}, \alpha} = & -\frac{2J_1}{N} \sum_{\mathbf{k}} \left(\cos \left(k_x - \frac{q_x}{2} \right) + \cos(k_y) \right) \langle d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\
 \Delta_{\mathbf{q}, d_{x^2-y^2}, \alpha} = & -\frac{2J_1}{N} \sum_{\mathbf{k}} \left(\cos \left(k_x - \frac{q_x}{2} \right) - \cos(k_y) \right) \langle d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\
 \Delta_{\mathbf{q}, s_{x^2y^2}, \alpha} = & -\frac{8J_2}{N} \sum_{\mathbf{k}} \cos \left(k_x - \frac{q_x}{2} \right) \cos(k_y) \langle d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle \\
 \Delta_{\mathbf{q}, d_{xy}, \alpha} = & -\frac{8J_2}{N} \sum_{\mathbf{k}} \sin \left(k_x - \frac{q_x}{2} \right) \sin(k_y) \langle d_{\alpha, -\mathbf{k} + \mathbf{q}, \downarrow} d_{\alpha, \mathbf{k}, \uparrow} \rangle
 \end{aligned} \tag{3.3.4}$$

And the additional term $C_{\mathbf{q}}(\phi)$ in equation (3.3.2) is given by:

$$C_{\mathbf{q}}(\phi) = \sum_{\alpha, \mathbf{k}} \left(\frac{N}{2J_1} |\Delta_{\mathbf{q}, s_{x^2+y^2}, \alpha}|^2 + \frac{N}{2J_1} |\Delta_{\mathbf{q}, d_{x^2-y^2}, \alpha}|^2 + \frac{N}{8J_2} |\Delta_{\mathbf{q}, s_{x^2y^2}, \alpha}|^2 + \frac{N}{8J_2} |\Delta_{\mathbf{q}, d_{xy}, \alpha}|^2 \right) \tag{3.3.5}$$

In order to solve the set of self-consistency equations (3.3.4), we need to diagonalize the Hamiltonian. Following the procedure outlined in the previous chapter, we start writing

the Hamiltonian in the matrix form $H_{\mathbf{q}}(\phi) = \sum_{\mathbf{k}} \Psi_{\mathbf{q}}(\mathbf{k})^\dagger A_{\mathbf{q}}(\mathbf{k}, \phi) \Psi_{\mathbf{q}}(\mathbf{k}) + C_{\mathbf{q}}(\phi)$, where $\Psi_{\mathbf{q}}(\mathbf{k})^\dagger = (d_{x,\mathbf{k},\uparrow}^\dagger, d_{x,-\mathbf{k}+\mathbf{q},\downarrow}, d_{y,\mathbf{k},\uparrow}^\dagger, d_{y,-\mathbf{k}+\mathbf{q},\downarrow})$, and the matrix $A_{\mathbf{q}}(\mathbf{k}, \phi)$ is given by:

$$A_{\mathbf{q}}(\mathbf{k}, \phi) = \begin{pmatrix} \epsilon_x(\mathbf{k} - \phi\hat{x}) & \Delta_{\mathbf{q},x}(\mathbf{k}) & \epsilon_{xy}(\mathbf{k} - \phi\hat{x}) & 0 \\ \Delta_{\mathbf{q},x}(\mathbf{k})^* & -\epsilon_x(-\mathbf{k} + \mathbf{q} - \phi\hat{x}) & 0 & -\epsilon_{xy}(-\mathbf{k} + \mathbf{q} - \phi\hat{x}) \\ \epsilon_{xy}(\mathbf{k} - \phi\hat{x}) & 0 & \epsilon_y(\mathbf{k} - \phi\hat{x}) & \Delta_{\mathbf{q},y}(\mathbf{k}) \\ 0 & -\epsilon_{xy}(-\mathbf{k} + \mathbf{q} - \phi\hat{x}) & \Delta_{\mathbf{q},y}(\mathbf{k})^* & -\epsilon_y(-\mathbf{k} + \mathbf{q} - \phi\hat{x}) \end{pmatrix} \quad (3.3.6)$$

Next, we find a unitary transformation $U_{\mathbf{q}}(\mathbf{k}, \phi)$ that diagonalizes the matrix $A_{\mathbf{q}}(\mathbf{k}, \phi)$, i.e. $A_{\mathbf{q}}(\mathbf{k}, \phi) = U_{\mathbf{q}}(\mathbf{k}, \phi) E_{\mathbf{q}}(\mathbf{k}, \phi) U_{\mathbf{q}}(\mathbf{k}, \phi)^\dagger$ with $E_{\mathbf{q}}(\mathbf{k}, \phi)$, a diagonal matrix whose entries are the eigenvalues of $A_{\mathbf{q}}(\mathbf{k}, \phi)$. In terms of these matrices, the averages that enter the self-consistency equations (3.3.4) become:

$$\begin{aligned} \langle d_{x,-\mathbf{k}+\mathbf{q},\downarrow} d_{x,\mathbf{k},\uparrow} \rangle &= \sum_n (U_{\mathbf{q}}(\mathbf{k}, \phi))_{2,n}^* (U_{\mathbf{q}}(\mathbf{k}, \phi))_{1,n} f((E_{\mathbf{q}}(\mathbf{k}, \phi))_n) \\ \langle d_{y,-\mathbf{k}+\mathbf{q},\downarrow} d_{y,\mathbf{k},\uparrow} \rangle &= \sum_n (U_{\mathbf{q}}(\mathbf{k}, \phi))_{4,n}^* (U_{\mathbf{q}}(\mathbf{k}, \phi))_{3,n} f((E_{\mathbf{q}}(\mathbf{k}, \phi))_n) \end{aligned} \quad (3.3.7)$$

Since we will be working at zero temperature, as in the previous chapter, $f(E) = 1 - \Theta(E)$.

We now have all the information needed to obtain a numerical solution of the self-consistency equations for each of the possible values of $\mathbf{q}$. Then we select the ground state of the system by choosing the value of $\mathbf{q}$ that minimizes the energy. We find the energy of a given $\mathbf{q}$ pairing momentum configuration in terms of the eigenvalues of the $A_{\mathbf{q}}(\mathbf{k}, \phi)$ matrices.

$$E_{\mathbf{q}}(\phi) = \langle H_{\mathbf{q}}(\phi) \rangle = \sum_{\mathbf{k},n} (E_{\mathbf{q}}(\mathbf{k}, \phi))_n f((E_{\mathbf{q}}(\mathbf{k}, \phi))_n) + C_{\mathbf{q}}(\phi) \quad (3.3.8)$$

Comparing Figure 3.7 with Figure 2.3, we can see that the the energy dependence on flux is, as expected, qualitatively the same for both the $s_{\pm}$ -wave loop and the s -wave loop.

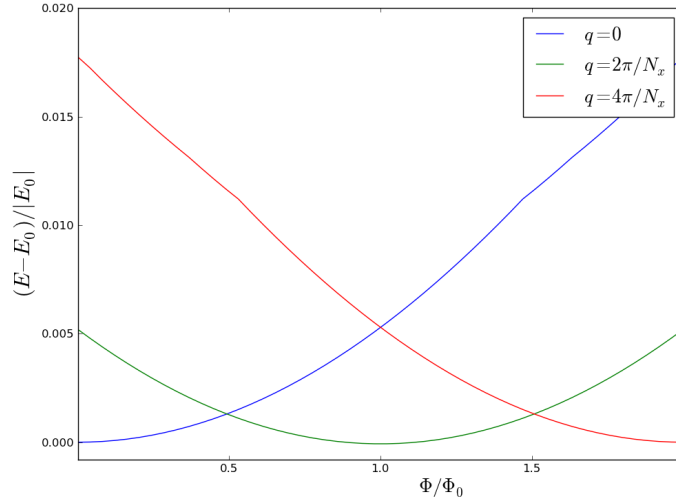


Figure 3.7: Energy dependence on flux for $J_2 = 2$, $J_1 = 0.5$, $\mu = 1.8$, $N_x = 16$, $N_y = 16$ at zero temperature.

This energy-flux relation is independent of our decision to bend the loop in the x -direction. This can be verified easily by analysing the behaviour of the loop with $t_1 \rightarrow t_2$ and $t_2 \rightarrow t_1$. In such case, we find an energy dependence on flux similar to the one shown in Figure 3.7. Furthermore, the qualitative behaviour of the energy-flux relation in the zones of the phase diagram where the $s_{x^2+y^2}$ pairing symmetry is dominant is the same.

3.4 Discussion

In this chapter, we introduced the model that will be used to describe the iron-pnictide part of the composite loop in the next chapter. The model allows pairing with four possible symmetries: $s_{x^2+y^2} \sim \cos(k_x) + \cos(k_y)$, $d_{x^2-y^2} \sim \cos(k_x) - \cos(k_y)$, $s_{x^2y^2} \sim \cos(k_x) \cos(k_y)$, and $d_{xy} \sim \sin(k_x) \sin(k_y)$. We find that at zero temperature the pairing symmetry $s_{x^2y^2}$ dominates for a large part of the phase diagram. In the parts of the phase diagram where the pairing symmetry $s_{x^2y^2}$ is sufficiently dominant, the order parameter has $s_{\pm}$ symmetry, i.e. changes sign between the electron and hole pockets of the Fermi surface. Hence,

we have shown that for the correct choice of parameters this model results in the pairing symmetry we are interested in describing.

In addition, we have studied the effect of adding flux to this model using self-consistent mean field theory. As in the previous chapter, we used an ansatz which assumed that all Cooper pairs had the same center of mass momentum. We find that the energy-flux relation is periodic with flux quantum $hc/2e$ period and has minima at integer flux quantum values. Also, the pair momenta $\mathbf{q}$ which corresponds to the ground state of the system has the same dependence in flux as found for the s -wave loop. Therefore, under the assumption of having a single pair momenta, the behaviour of the $s_{\pm}$ loop is essentially the same as that of the s -wave loop.

Composite loop

After studying the effect of threading an s -wave superconductor loop and an iron-pnictide superconductor loop with magnetic flux, we can now proceed to study the behaviour of a flux threaded composite loop. In this chapter, we will be working with the arrangement shown in Figure 4.1. The arrangement consists of an iron-pnictide superconductor and an s -wave superconductor joined by two Josephson junctions forming a loop that is threaded with flux. We have N_y lattice sites in the y -direction, N_x sites in the x -direction in the iron-pnictide superconductor, and N_{xs} sites on the s -wave superconductor. Sites whose x coordinate goes from 1 to N_x correspond to lattice sites in the iron-pnictide superconductor, while sites whose x coordinate ranges from $N_x + 1$ to $N_x + N_{xs}$ belong to the s -wave superconductor. We will use the models developed in the previous two chapters to model the s -wave superconductor and the iron-pnictide superconductor. For simplicity, we will consider periodic boundary conditions on the y -direction, and that the two superconductors have the same lattice constant which we will set to 1.

The Hamiltonian for the composite loop is given by:

$$H = H_s + H_{pn} + H_{junc} \quad (4.0.1)$$

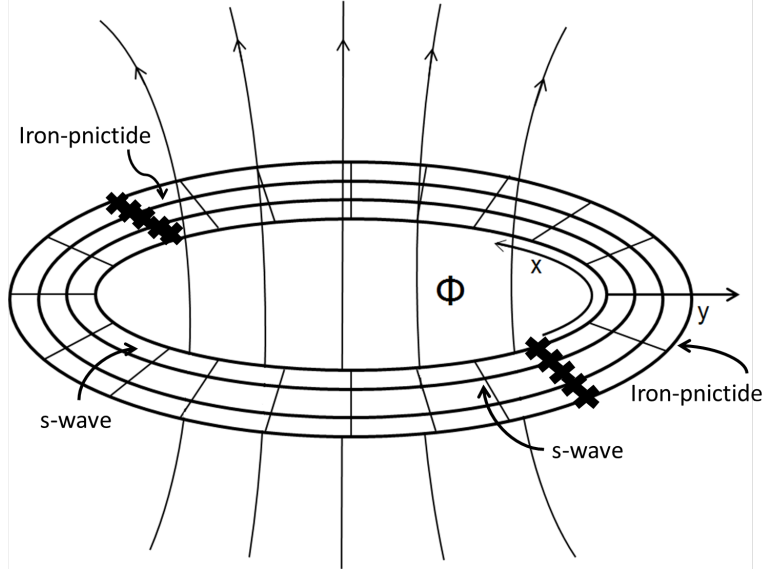


Figure 4.1: *s*-wave/iron-pnictide composite loop.

We will describe the junctions through four hopping parameters $t_{1\alpha}$ and $t_{2\alpha}$ ($\alpha = x, y$), which give the probability for the electron on the *s*-wave superconductor to hop to the $d_{\alpha z}$ orbital in the first and second junction. The hopping amplitudes $t_{1\alpha}$ and $t_{2\alpha}$ have a smaller magnitude than the hopping amplitudes for both the *s*-wave superconductor and the iron-pnictide superconductor. We proceed to write H_{junc} in real space for zero magnetic flux as:

$$H_{junc} = \sum_{n,\alpha} \left(-t_{1\alpha} d_{\alpha}^{\dagger}(1, n) c(N_x + N_{xs}, n) - t_{1\alpha} c^{\dagger}(N_x + N_{xs}, n) d_{\alpha}(1, n) \right. \\ \left. - t_{2\alpha} d_{\alpha}^{\dagger}(N_x, n) c(N_x + 1, n) - t_{2\alpha} c^{\dagger}(N_x + 1, n) d_{\alpha}(N_x + 1, n) \right) \quad (4.0.2)$$

We add the effect of the magnetic flux in $H_{junction}$ in the same way as in previous chapters, through Peierls substitution, obtaining:

$$H_{junc} = \sum_{n,\alpha} \left(-t_{1\alpha} e^{-i\phi} d_{\alpha}^{\dagger}(1, n) c(N_x + N_{xs}, n) - t_{1\alpha} e^{i\phi} c^{\dagger}(N_x + N_{xs}, n) d_{\alpha}(1, n) \right. \\ \left. - t_{2\alpha} e^{i\phi} d_{\alpha}^{\dagger}(N_x, n) c(N_x + 1, n) - t_{2\alpha} e^{-i\phi} c^{\dagger}(N_x + 1, n) d_{\alpha}(N_x, n) \right) \quad (4.0.3)$$

Since the total number of ions in the x -direction is equal to $N_x + N_{xs}$, the phase ϕ in the above equation is given by $\phi = \frac{\pi}{N_x + N_{xs}} \frac{\Phi}{\Phi_0}$.

4.1 Mixed real and momentum space description

By adding the two junctions to the system, we have broken the discrete translational invariance in the x -direction. Therefore k_x is no longer a good quantum number, however k_y still is. Bearing this in mind, we find that the most useful way to write down the Hamiltonian for the system is in terms of a mixed real and momentum space description. The operators in this description can be obtained by taking a Fourier transform of the real space operators, but only on the y -direction, i.e., we define $c_{k_y, \sigma}(m)$, $d_{x, k_y, \sigma}(m)$ and $d_{y, k_y, \sigma}(m)$ as:

$$\begin{aligned} c_{\sigma}(\mathbf{r}) &= c_{\sigma}(m, n) = \frac{1}{\sqrt{N_y}} \sum_{k_y} c_{k_y, \sigma}(m) e^{-i n k_y} \\ d_{\alpha, \sigma}(\mathbf{r}) &= d_{\alpha, \sigma}(m, n) = \frac{1}{\sqrt{N_y}} \sum_{k_y} d_{\alpha, k_y, \sigma}(m) e^{-i n k_y} \end{aligned} \quad (4.1.1)$$

The operator $c_{k_y, \sigma}(m)$ annihilates an electron with momentum k_y and spin σ in the orbital of an ion with x -coordinate m in the s -wave superconductor. Analogously, the operator $d_{\alpha, k_y, \sigma}(m)$ annihilates an electron with momentum k_y and spin σ in the orbital α of an ion with x -coordinate m in the iron pnictide superconductor.

4.1.1 s -wave superconductor

The Hamiltonian for the s -wave superconducting loop obtained in section 2.2 can be written in terms of the half-Fourier transformed operators defined by equation (4.1.1) as:

$$H_s = \sum_{k_y, \sigma} c_{\sigma}^{\dagger}(k_y) K_c(k_y, \phi) c_{\sigma}(k_y) + \sum_{k_y} \left(c_{\uparrow}^{\dagger}(k_y) \Delta_c (c_{\downarrow}^{\dagger}(-k_y))^T + (c_{\downarrow}(-k_y))^T \Delta_c^{\dagger} c_{\uparrow}(k_y) \right) + C_s(\phi) \quad (4.1.2)$$

In the above equation we have introduced a vector operator $c_\sigma^\dagger(k_y)$, which is defined as $c_\sigma^\dagger(k_y) = (c_{k_y,\sigma}^\dagger(1), c_{k_y,\sigma}^\dagger(2), \dots, c_{k_y,\sigma}^\dagger(N_{xs}))$. The kinetic part of the s -wave Hamiltonian is given by the matrices $K_c(k_y, \phi)$. They are tridiagonal and Hermitian matrices whose non-zero entries are given by:

$$\begin{aligned} (K_c(k_y, \phi))_{m,m} &= -2t_0 \cos(k_y) - \mu \\ (K_c(k_y, \phi))_{m,m+1} &= -t_0 e^{i\phi} \\ (K_c(k_y, \phi))_{m+1,m} &= (K_c(k_y, \phi))_{m,m+1}^* \end{aligned} \quad (4.1.3)$$

The matrix $\Delta_c(m)$ is diagonal and its entries $(\Delta_c)_{mm} = \Delta_c(m)$ give us the pairing amplitude for each x coordinate. These pairing amplitudes must be solutions of the self-consistency equations:

$$\Delta_c(m) = \frac{U}{N_y} \sum_{k_y} \langle c_{-k_y,\downarrow}(m) c_{k_y,\uparrow}(m) \rangle \quad (4.1.4)$$

Finally, $C_s(\phi)$ is given by:

$$C_s(\phi) = -\frac{N_y}{U} \sum_m |\Delta_c(m)|^2 \quad (4.1.5)$$

As a sanity check, we solved this self-consistency equations for the flux threaded s -wave superconducting loop. We solve the equation numerically using an iterative method starting with the ansatz $\Delta_c(m) \sim e^{-iqm}$, with $q = \frac{2\pi n}{N_{xs}}$ and n an integer between 0 and $N_{xs} - 1$. Using this ansatz, we obtain the same results as found in section 2.2.

4.1.2 Iron-pnictide superconductor

In terms of the mixed real and momentum space operators, the mean-field Hamiltonian for the flux threaded iron-pnictide superconductor loop may be written as:

$$\begin{aligned}
H_{pn} = & \sum_{k_y, \sigma, \alpha} (d_{\alpha, \sigma}^\dagger(k_y) K_\alpha(k_y) d_{\alpha, \sigma}(k_y) + d_{\alpha, \sigma}^\dagger(k_y) K_{xy}(k_y) d_{\bar{\alpha}, \sigma}(k_y)) \\
& + \sum_{k_y, \alpha} \left(d_{\alpha, \uparrow}^\dagger(k_y) \Delta_\alpha(k_y) (d_{\alpha, \downarrow}^\dagger(-k_y))^T + (d_{\alpha, \downarrow}(k_y))^T \Delta_\alpha^\dagger(k_y) (d_{\alpha, \downarrow}(-k_y)) \right) + C_{pn}(\phi)
\end{aligned} \tag{4.1.6}$$

Here $d_{\alpha, \sigma}^\dagger(k_y) = (d_{\alpha, k_y, \sigma}^\dagger(1), d_{\alpha, k_y, \sigma}^\dagger(2), \dots, d_{\alpha, k_y, \sigma}^\dagger(N_x))$, α as usual denotes the orbital and $\bar{\alpha}$ is the orbital opposite to α , i.e. $\bar{\alpha} = y$ if $\alpha = x$ and vice versa. The matrices $K_\alpha(k_y, \phi)$ contain the intra-orbital hopping terms and the matrices $K_\alpha(k_y, \phi)$, the inter-orbital hopping. These three types of matrices $K_x(k_y, \phi)$, $K_y(k_y, \phi)$, $K_{xy}(k_y, \phi)$ are Hermitian and its non-zero entries are:

$$\begin{aligned}
(K_x(k_y, \phi))_{m, m} &= -2t_2 \cos(k_y) - \mu \\
(K_x(k_y, \phi))_{m, m+1} &= -(t_1 + 2t_3 \cos(k_y)) e^{i\phi} \\
(K_y(k_y, \phi))_{m, m} &= -2t_1 \cos(k_y) - \mu \\
(K_y(k_y, \phi))_{m, m+1} &= -(t_2 + 2t_3 \cos(k_y)) e^{i\phi} \\
(K_{xy}(k_y, \phi))_{m, m+1} &= -2it_4 \sin(k_y) e^{i\phi}
\end{aligned} \tag{4.1.7}$$

The pairing structure of the mean field Hamiltonian for the iron-pnictide loop in each orbital is given by the matrices $(\Delta_\alpha(k_y))$, whose non-zero elements are:

$$\begin{aligned}
(\Delta_\alpha(k_y))_{mm} &= \cos(k_y) (\Delta_{s_{x^2+y^2}, \alpha}(m) - \Delta_{d_{x^2-y^2}, \alpha}(m)) \\
(\Delta_\alpha(k_y))_{m+1, m} &= \Delta_{s_{x^2+y^2}, \alpha}(m) + \Delta_{d_{x^2-y^2}, \alpha}(m) + \cos(k_y) \Delta_{s_{x^2+y^2}, \alpha}(m) - \sin(k_y) \Delta_{d_{xy}, \alpha}(m) \\
(\Delta_\alpha(k_y))_{m, m+1} &= \Delta_{s_{x^2+y^2}, \alpha}(m) + \Delta_{d_{x^2-y^2}, \alpha}(m) + \cos(k_y) \Delta_{s_{x^2+y^2}, \alpha}(m) + \sin(k_y) \Delta_{d_{xy}, \alpha}(m)
\end{aligned} \tag{4.1.8}$$

In the above set of equations we have introduced a set of pairing amplitudes in different channels in consistency with the previously solved momentum description. These pairing amplitudes satisfy the equations:

$$\begin{aligned}
\Delta_{s_{x^2+y^2},\alpha}(m) - \Delta_{d_{x^2-y^2},\alpha}(m) &= -\frac{4J_1}{N_y} \sum_{k_y} \cos(k_y) \langle d_{\alpha,-k_y,\downarrow}(m) d_{\alpha,k_y,\uparrow}(m) \rangle \\
\Delta_{s_{x^2+y^2},\alpha}(m) + \Delta_{d_{x^2-y^2},\alpha}(m) &= -\frac{J_1}{N_y} \sum_{k_y} (\langle d_{\alpha,-k_y,\downarrow}(m+1) d_{\alpha,k_y,\uparrow}(m) \rangle + \langle d_{\alpha,-k_y,\downarrow}(m) d_{\alpha,k_y,\uparrow}(m+1) \rangle) \\
\Delta_{s_{x^2y^2},\alpha}(m) &= -\frac{2J_2}{N_y} \sum_{k_y} \cos(k_y) (\langle d_{\alpha,-k_y,\downarrow}(m+1) d_{\alpha,k_y,\uparrow}(m) \rangle + \langle d_{\alpha,-k_y,\downarrow}(m) d_{\alpha,k_y,\uparrow}(m+1) \rangle) \\
\Delta_{d_{xy},\alpha}(m) &= -\frac{2J_2}{N_y} \sum_{k_y} \sin(k_y) (\langle d_{\alpha,-k_y,\downarrow}(m+1) d_{\alpha,k_y,\uparrow}(m) \rangle - \langle d_{\alpha,-k_y,\downarrow}(m) d_{\alpha,k_y,\uparrow}(m+1) \rangle)
\end{aligned} \tag{4.1.9}$$

We can write the flux dependent constant $C_{pn}(\phi)$ in terms of the different pairing amplitudes as:

$$\begin{aligned}
C_{pn}(\phi) &= \sum_{m,\alpha} \left(\frac{N_y}{4J_1} |\Delta_{s_{x^2+y^2},\alpha}(m) - \Delta_{d_{x^2-y^2},\alpha}(m)|^2 + \frac{N_y}{J_1} |\Delta_{s_{x^2+y^2},\alpha}(m) + \Delta_{d_{x^2-y^2},\alpha}(m)|^2 \right. \\
&\quad \left. + \frac{N_y}{2J_2} |\Delta_{s_{x^2y^2}}(m)|^2 + \frac{N_y}{2J_2} |\Delta_{d_{xy}}(m)|^2 \right)
\end{aligned} \tag{4.1.10}$$

As in the previous case, we can verify the Hamiltonian in equation (4.1.6) and the above self-consistency equations by using them to solve the same problem as in the previous chapter. We start by noting that a solution with a pairing momentum $\mathbf{q} = q\hat{x}$, has the next form in the mixed real and momentum space description:

$$\begin{aligned}
\Delta_{s_{x^2+y^2},\alpha}(m) - \Delta_{d_{x^2-y^2},\alpha}(m) &= \frac{1}{2} (\Delta_{\mathbf{q},s_{x^2+y^2},\alpha} - \Delta_{\mathbf{q},d_{x^2-y^2},\alpha}) e^{-iqm} \\
\Delta_{s_{x^2+y^2},\alpha}(m) + \Delta_{d_{x^2-y^2},\alpha}(m) &= \frac{1}{4} (\Delta_{\mathbf{q},s_{x^2+y^2},\alpha} + \Delta_{\mathbf{q},d_{x^2-y^2},\alpha}) e^{-iqm} e^{-iq/2} \\
\Delta_{s_{x^2y^2},\alpha}(m) &= \frac{1}{2} \Delta_{\mathbf{q},s_{x^2y^2},\alpha} e^{-iqm} e^{-iq/2} \\
\Delta_{d_{xy},\alpha}(m) &= \frac{i}{2} \Delta_{\mathbf{q},d_{xy},\alpha} e^{-iqm} e^{-iq/2}
\end{aligned} \tag{4.1.11}$$

We can solve the self-consistency equations iterating from a starting point in which all the pairing amplitudes have same the space dependence than in the above equation. The solution found following in this description is the same as the one found in section 3.3.

4.1.3 Junction

We can also rewrite $H_{junc}(\phi)$ in terms of the vector operators $c_\sigma^\dagger(k_y)$ and $d_{\alpha,\sigma}^\dagger(k_y)$, which have been defined in the two previous sections as:

$$H_{junc}(\phi) = \sum_{k_y, \sigma} (d_{\alpha, \sigma}^\dagger(k_y) T_\alpha(\phi) c_\sigma(k_y) + c_\sigma^\dagger(k_y) T_\alpha(\phi)^\dagger d_{\alpha, \sigma}(k_y)) \quad (4.1.12)$$

The matrices $T_\alpha(\phi)$ from the above equation have only two non-zero elements which are given by:

$$\begin{aligned} (T_\alpha(\phi))_{1, N_x} &= -t_{2\alpha} e^{i\phi} \\ (T_\alpha(\phi))_{N_{xs}, 1} &= -t_{1\alpha} e^{-i\phi} \end{aligned} \quad (4.1.13)$$

4.1.4 Composite loop Hamiltonian

We now can put together different parts of the composite loop Hamiltonian, and write our mean field Hamiltonian as matrix plus a flux dependent constant.

$$H(\phi) = H_s + H_{pn} + H_{junc} = \sum_{k_y} \Psi(k_y)^\dagger A(k_y, \phi) \Psi(k_y) + C(\phi) \quad (4.1.14)$$

Where $\Psi(k_y)^\dagger = \left(d_{x,\uparrow}^\dagger(k_y), (d_{x,\downarrow}(-k_y))^T, d_{y,\uparrow}^\dagger(k_y), (d_{y,\downarrow}(-k_y))^T, c_\uparrow^\dagger(k_y), (c_\downarrow(-k_y))^T \right)$, the constant $C(\phi)$ is equal to $C_s(\phi) + C_{pn}(\phi)$, and the matrix $A(k_y, \phi)$ is given by:

$$A(k_y, \phi) = \begin{pmatrix} K_x(k_y, \phi) & \Delta_x(k_y) & K_{xy}(k_y, \phi) & 0 & T_x(\phi) & 0 \\ \Delta_x(k_y)^\dagger & -K_x(k_y, \phi)^* & 0 & K_{xy}(k_y, \phi)^* & 0 & -T_x(\phi)^* \\ K_{xy}(k_y, \phi) & 0 & K_y(k_y, \phi) & \Delta_y(k_y) & T_y(\phi) & 0 \\ 0 & K_{xy}(k_y, \phi)^* & \Delta_y(k_y)^\dagger & -K_y(k_y, \phi)^* & 0 & -T_y(\phi)^* \\ T_x(\phi)^\dagger & 0 & T_y(\phi)^\dagger & 0 & K_c(k_y, \phi) & \Delta_c \\ 0 & -T_x(\phi)^T & 0 & -T_y(\phi)^T & \Delta_c^\dagger & -K_c(k_y, \phi)^* \end{pmatrix} \quad (4.1.15)$$

Following the procedure outlined in the previous chapters, we proceed to find a set of unitary transformations $U(k_y, \phi)$ that diagonalize the matrices $A(k_y, \phi)$, i.e. a transformation $U(k_y, \phi)$ such that $A(k_y, \phi) = U(k_y, \phi)E(k_y, \phi)U^\dagger(k_y, \phi)$, with $E(k_y, \phi)$ a diagonal matrix. In terms of these unitary transformations, the averages that enter the self-consistency equations (4.1.4) and (4.1.9) are given by:

$$\begin{aligned} \langle d_{x,-k_y,\downarrow}(m)d_{x,k_y,\uparrow}(n) \rangle &= \sum_l (U(k_y, \phi))_{N_x+m,l}^* (U(k_y, \phi))_{n,l} f(E_l(k_y, \phi)) \\ \langle d_{y,-k_y,\downarrow}(m)d_{y,k_y,\uparrow}(n) \rangle &= \sum_l (U(k_y, \phi))_{3N_x+m,l}^* (U(k_y, \phi))_{2N_x+n,l} f(E_l(k_y, \phi)) \\ \langle c_{-k_y,\downarrow}(m)c_{k_y,\uparrow}(m) \rangle &= \sum_l (U(k_y, \phi))_{4N_x+N_{xs}+m,l}^* (U(k_y, \phi))_{4N_x+m,l} f(E_l(k_y, \phi)) \end{aligned} \quad (4.1.16)$$

And the mean-field energy by:

$$E(\phi) = \langle H(\phi) \rangle = \sum_{k_y, l} E_l(k_y, \phi) f(E_l(k_y, \phi)) + C(\phi) \quad (4.1.17)$$

4.2 Preliminary Results

Now that we have laid down the formalism to treat the composite loop, we need to find solutions to the self-consistency equations (4.1.4) and (4.1.9) that minimize the energy given by equation (4.1.17). We are particularly interested in finding an energy-flux relation in the “double minimum” regime predicted by the modified Ginzburg-Landau model (see section 1.6). Unfortunately, the system formed by this set of equations has many possible solutions. Since we are using an iterative method to solve them, the solution depends largely on the initial set of conditions from which we start iterating. Therefore, whether we are able to find the behaviour we are interested in does not only depends on the microscopic parameters of the model, but also on our ability to set the right initial conditions.

4.2.1 Composite loop between two *s*-wave superconductors

In order to gain some intuition on the problem, we started by solving a composite loop between two *s*-wave superconductors. Since we have a superconducting loop, we expect the energy dependence on flux to be periodic with a flux quantum period in the thermodynamic limit. Hence, we focus on studying the system for flux between 0 and Φ_0 . We picked the initial conditions following the spatial dependence found for the *s*-wave loop, i.e. $\Delta_c(m) \sim e^{-iqm}$, with $q = 0$ and $q = 2\pi/(N_{x_1} + N_{x_2})$, where N_{x_1} and N_{x_2} are the number of ions in the *x*-direction in each of the superconductors that form the composite loop.

Iterating with the initial condition of a constant order parameter leads to the solution shown in Figure 4.2. The magnitude of the order parameter $\Delta_c(m)$ does not exhibit a strong dependence on flux. Thus, we chose to plot $|\Delta_c(m)|$ for only one value of flux. We can see in Figure 4.2a that $|\Delta_c(m)|$ is greater at the junctions, it fluctuates near the junction, and it is almost constant far from the junction. This behaviour is maintained for all the

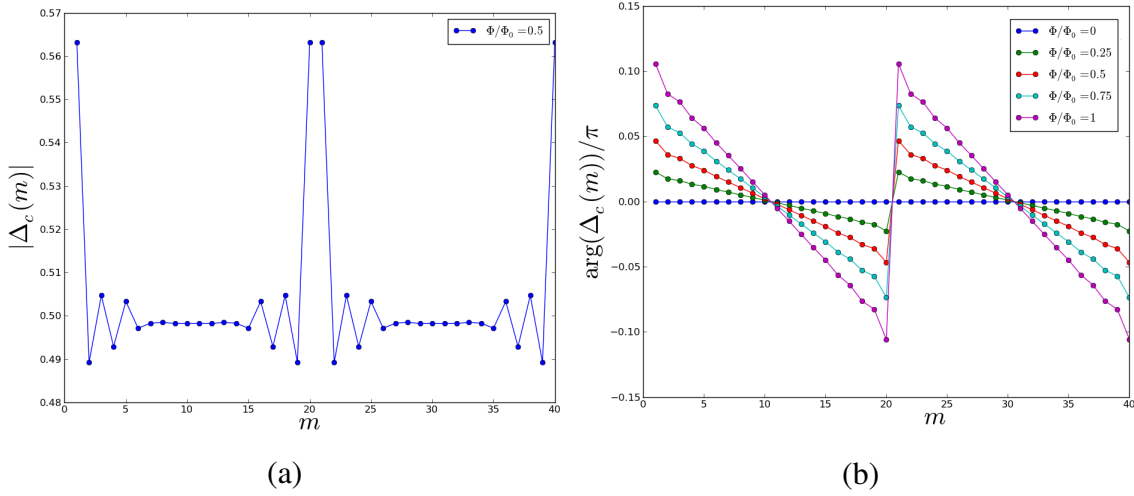


Figure 4.2: Solution 1. Spatial dependence of the order parameter for a composite loop between two s -wave superconductors iterating with a constant order parameter as the starting point at $T = 0$. The choice of parameters is $t_0 = 1$, $U = -3$, $\mu = 1.8$, and the hopping amplitude in both junctions is 0.5. (a) Magnitude of the order parameter for $\Phi = \Phi_0/2$. Note that the order parameter amplitude is almost constant on the loop sites. (b) Phase of the order parameter for different values of the flux.

values of flux between 0 and Φ_0 with very slight changes in the magnitude. The phase of $\Delta_c(m)$ displayed in Figure 4.2b exhibits a more interesting behaviour. Contrary to the case of an s -wave loop, where there was a constant phase jump between one site and the next one ($\Delta_c(m) \sim e^{-iqm}$), we now find that most of the phase difference occurs at the junctions. In Figure 4.2b we can see that the change in phase at the two junctions is the same. We will refer to the spatial dependence of the order parameter discussed in this paragraph as “Solution 1”.

“Solution 2” is found by iterating with $\Delta_c(m) \sim e^{-iqm}$ for $q = 2\pi/(N_{x_1} + N_{x_2})$ as the starting point. The spatial dependence of the order parameter $\Delta_c(m)$ for this solution appears in Figure 4.3. We found that the magnitude of the order parameter is exactly the same as in Solution 1. However, the phase of the order parameter shows a very different behaviour. The phase difference between the two different ends of each superconductor increases with the flux as in Solution 1. This phase difference is close to π in contrast to Solution 1 where this phase difference is about ten times smaller.

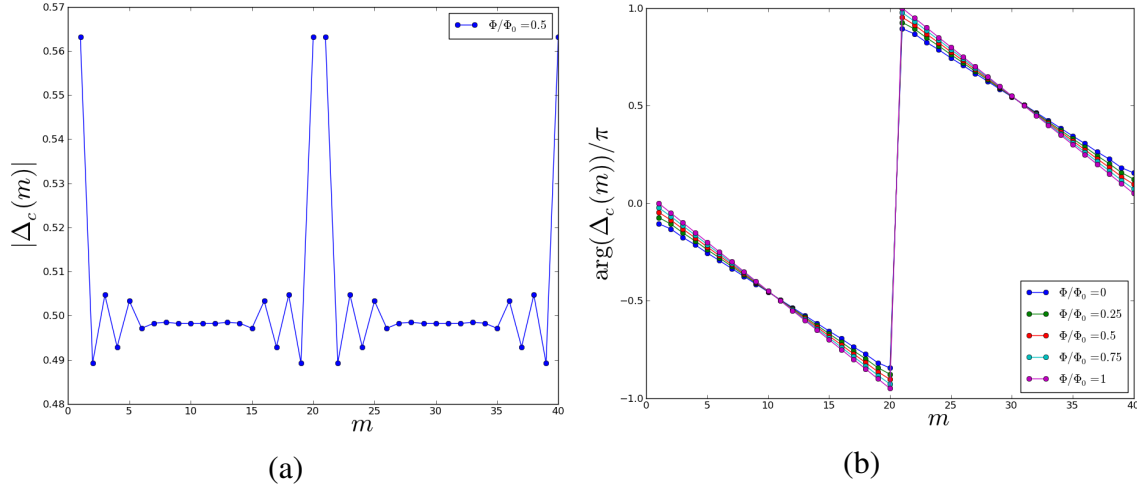


Figure 4.3: Solution 2. Spatial dependence of the order parameter for a composite loop between two s -wave superconductors iterating with $\Delta_c(m) \sim e^{-iqm}$ for $q = 2\pi/(N_{x_1} + N_{x_2})$ as the starting point at $T = 0$. The choice of parameters is $N_x = N_{x_s} = N_y = 20$, $t_0 = 1$, $U = -3$, $\mu = 1.8$, and the hopping amplitude in both junctions is 0.5. (a) Modulus of the order parameter for $\Phi = \Phi_0/2$. (b) Phase of the order parameter for different values of the flux.

One striking feature of Figures 4.2 and 4.3 is that the magnitude of the order parameter spikes just before the junction. The order parameter vanishes at the normal region (between sites 20 and 21 and between sites 40 and 1); hence we would expect the magnitude of the order parameter to decrease before the junction (at sites 20, 21, 40 and 1). This is not the behaviour observed in Figures 4.2 and 4.3. At present, we have found that, within our model, for large enough μ we obtain the expected behaviour, i.e. the magnitude of the order parameter decreases just before the junction. However, for small values of μ , we found that the order parameter spikes just before the junction, as can be seen in Figures 4.2 and 4.3. The cause of these two distinct behaviours remains unclear for us and will be a part of our future research.

Figure 4.4, shows the dependence of the mean-field energy on flux for each of the two solutions found. For flux between 0 and $\Phi_0/2$ the ground state of the system is given by Solution 1, while, for values of the flux between $\Phi_0/2$ and Φ_0 , it is given by Solution 2. The energy-flux relation for this system is similar to the ones found in the previous chapters.

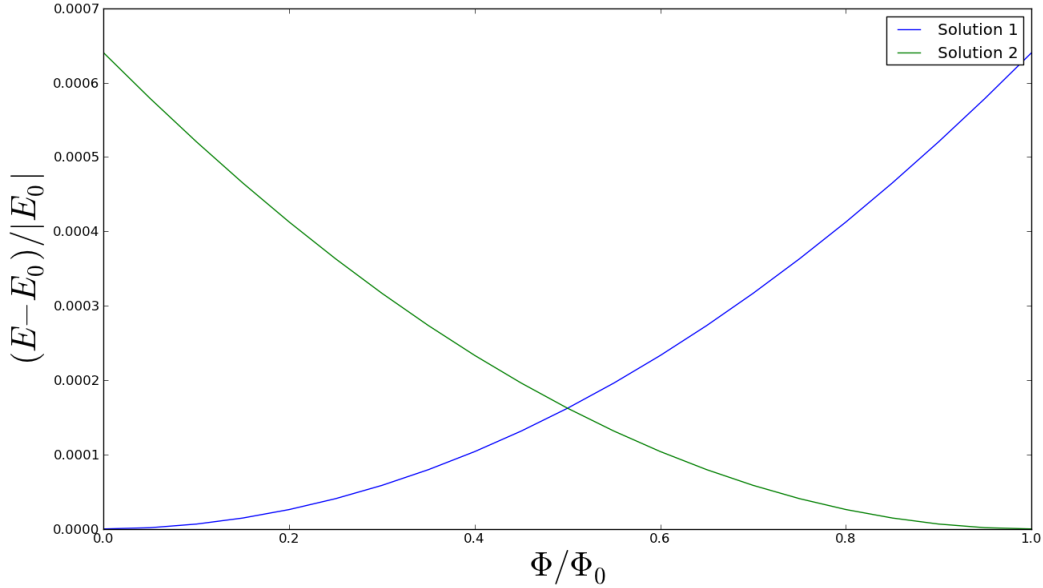


Figure 4.4: Energy dependence on flux for the two types of solutions found for the composite loop between two s -wave superconductors at $T = 0$ for $N_x = N_{xs} = N_y = 20$, $t_0 = 1$, $U = -3$, and $\mu = 1.8$, when the hopping amplitude in both junctions is equal to 0.5. E_0 is the energy at zero flux.

4.2.2 s -wave/iron-pnictide composite loop

For the s -wave/iron-pnictide composite loop, we have also found two different types of solutions by iterating the self-consistency equations (4.1.9) and (4.1.4), which we will call Solution 1 and Solution 2. In order to find Solution 1, one must start by setting an order parameter with constant phase. This initial guess is consistent with both the spatial behaviour of the solution found for the single s -wave loop at values of flux roughly between 0 and $\Phi_0/2$, and with Solution 1 for the s -wave/ s -wave composite loop where the change in phase is in general small. Solution 2 can be found by using two different initial guesses: 1) an order parameter where all the Cooper pairs have the same momentum $\mathbf{q} = q\hat{x}$ with $q = 2\pi/(N_{x_1} + N_{x_2})$; and 2) setting the initial phase difference in the order parameter between the end points of each superconductor to π .

We start by discussing the behaviour of the magnitudes of the different pairing ampli-

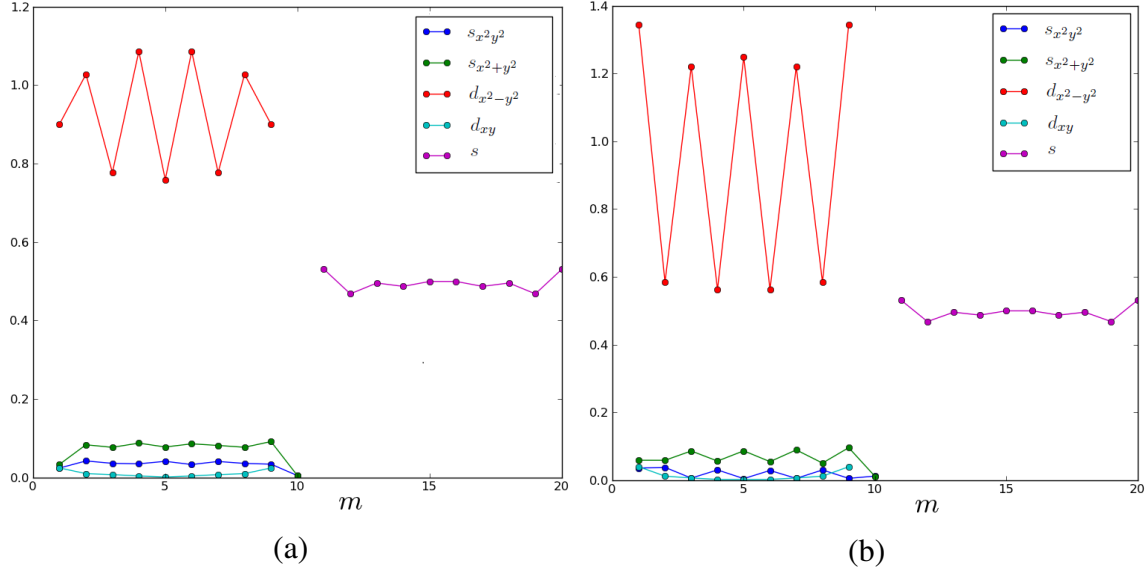


Figure 4.5: Spatial dependence of the magnitude of the different pairing amplitudes for Solution 1 in the composite iron-pnictide/s-wave loop for (a) the d_{xz} orbital and (b) the d_{yz} orbital at zero flux and zero temperature. The choice of parameters is $N_x = N_{xs} = N_y = 10$, $t_0 = 1$, $U = -3$, $\mu = \mu_s = 1.8$, $J_2 = 2$, $J_1 = 1$ and $t_{1x} = t_{1y} = t_{2x} = t_{2y} = 0.5$.

tudes in Solution 1 and Solution 2. As in the s -wave/ s -wave composite loop, the magnitudes of the pairing amplitudes are not strongly dependent on flux. For this reason, we choose only to plot the behaviour of the pairing amplitudes only for zero flux in Figures 4.5 and 4.6. We can see in the Figures that the pairing symmetry $s_{x^2y^2}$ dominates over the other pairing symmetries in the iron-pnictide part of the loop. This means that the order parameter in the iron-pnictide part of the loop has the symmetry that we are interested in, i.e. $s_{\pm}$. We can also notice that the magnitude of the order parameters on both solutions are very similar, although, contrary to the s -wave/ s -wave composite loop solutions, they are not identical. In addition for both cases the magnitude of the order parameter is larger for the d_{yz} orbital than for the d_{xz} orbital. This difference is due to the fact that the total number of ions in the y -direction is half the total number of ions in the x -direction. One last thing we can note from Figures 4.5 and 4.6 is that we find more oscillations in the magnitude of the different pairing amplitudes than in the s -wave/ s -wave loop, this is probably due to the

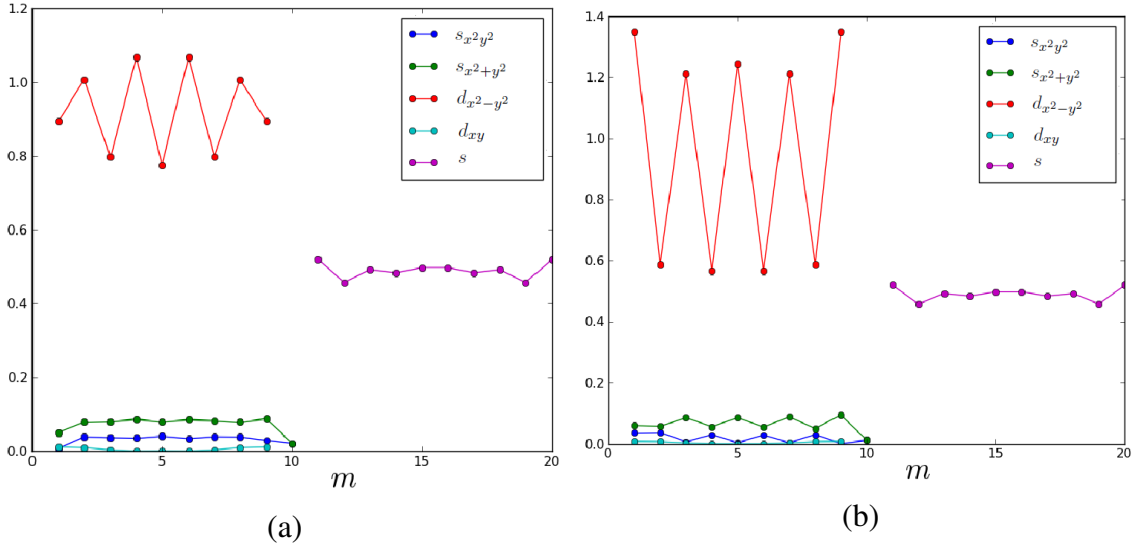


Figure 4.6: Spatial dependence of the magnitude of different pairing amplitudes for Solution 2 in the composite iron-pnictide/s-wave loop for (a) the d_{xz} orbital and (b) the d_{yz} orbital at zero flux and zero temperature. The choice of parameters is $N_x = N_{xs} = N_y = 10$, $t_0 = 1$, $U = -3$, $\mu = \mu_s = 1.8$, $J_2 = 2$, $J_1 = 1$ and $t_{1x} = t_{1y} = t_{2x} = t_{2y} = 0.5$.

smaller size of the system.

The spatial dependence of the phase of the $s_{x^2y^2}$ pairing symmetry in the pnictide part of the loop and the order parameter in the s -wave part of the loop are shown in Figure 4.7 for the two solutions found. The spatial dependence on phase in Solution 1 for the iron-pnictide/ s -wave loop is very similar to the one found for Solution 1 in the s -wave/ s -wave loop. However, the difference in order parameter phase between the two end points of each part of the loop is much higher in the iron-pnictide/ s -wave loop than in the s -wave/ s -wave loop. The differences in the phase's spatial dependence in Solution 2 between the two composite loops are more striking, especially the one corresponding to the behaviour at zero flux. As mentioned before, in Solution 2 for the s -wave/ s -wave loop there is a difference in phase close to π between the end points of each part of the loop, even at zero flux. In Solution 2 for the iron-pnictide/ s -wave loop, we found instead that at zero flux there is no phase difference between the end points of the superconductor, and that there are π jumps in each junction.

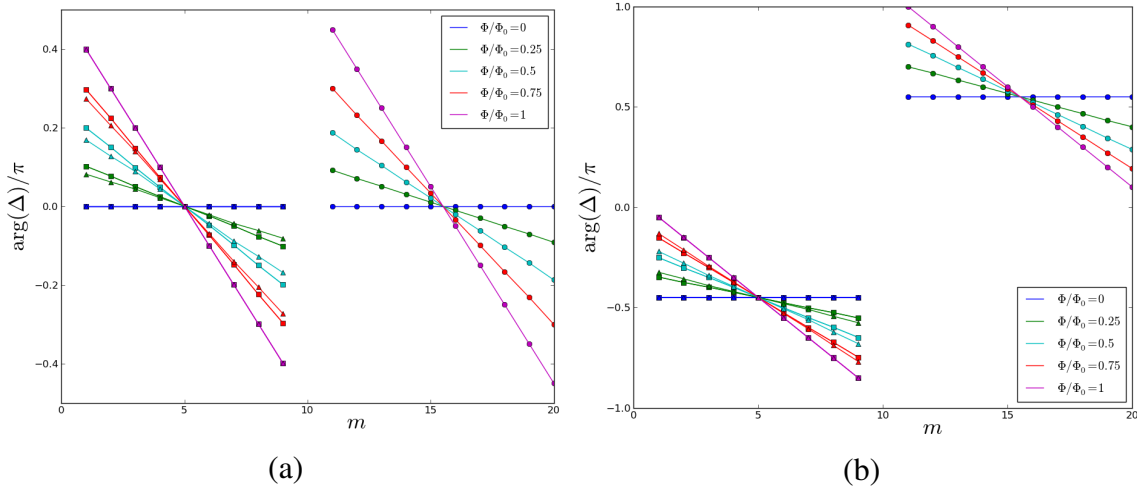


Figure 4.7: Spatial dependence of the phase of the pairing amplitudes: $\Delta_{s_{x^2y^2},x}(m)$, in squares, $\Delta_{s_{x^2y^2},y}(m)$, in triangles, and $\Delta_c(m)$, in circles, for (a) Solution 1 and (b) Solution 2 in the composite iron-pnictide/ s -wave loop at $T = 0$. The choice of parameters is $N_x = N_y = 10$, $t_0 = 1$, $U = -3$, $\mu = \mu_s = 1.8$, $J_2 = 2$, $J_1 = 1$ and $t_{1x} = t_{1y} = t_{2x} = t_{2y} = 0.5$.

Figure 4.8 depicts the energy-flux relation for Solution 1 and Solution 2. We find again an overall energy-flux relation with minima at 0 and Φ_0 and a maximum at $\Phi_0/2$. For values of the flux between 0 and $\Phi_0/2$, Solution 1 is favoured; while for values of flux between $\Phi_0/2$, and Φ_0 the energy is minimized by Solution 2.

As mentioned in section 1.6, the composite loop has already been studied a Ginzburg-Landau type formalism [53]. They found three possible regimes distinguished by the qualitative behaviour of the energy-flux relation: “time reversal breaking”, “single minimum” and “double minimum”. We are interested in finding an energy flux dependence in the “double minimum” regime, which would have a local minima at $\Phi_0/2$. This is not the behaviour shown in Figure 4.8. This can be due to two possible reasons: 1) there is no “double minimum” behaviour for the set of parameters used, or 2) we have not found the right initial set of conditions from which to start the iteration.

In the two solutions found both orbitals follow roughly the same qualitative behaviour. In order to interpret these solutions, we need to remember that the order parameter in the

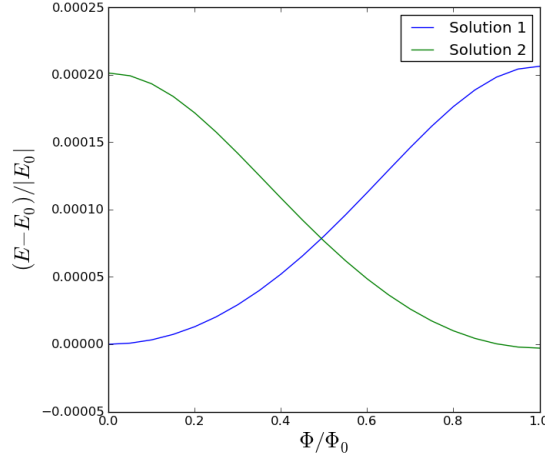


Figure 4.8: Energy dependence on flux for the two types of solutions found for the composite iron-pnictide/ s -wave loop at $T = 0$. E_0 is the energy at zero flux. The choice of parameters is $N_x = N_{xs} = N_y = 10$, $t_0 = 1$, $U = -3$, $\mu = \mu_s = 1.8$, $J_2 = 2$, $J_1 = 1$ and $t_{1x} = t_{1y} = t_{2x} = t_{2y} = 0.5$.

iron-pnictide part of the loop has $s_{\pm}$ symmetry, which means that there is a phase difference of π between the order parameter in hole and in electron pockets. The order parameter in the hole pockets has the same phase as the pairing amplitude while the phase in the electron pockets is π shifted. Hence, we interpret the solutions as follows: for flux between 0 and $\Phi_0/2$ the order parameter in hole pockets follows the behaviour exhibited in 4.7a, and the order parameter in electron pockets the one in 4.7b; for flux between $\Phi_0/2$ and Φ_0 we have the the order parameter in hole pockets follows the behaviour exhibited in 4.7b, and the order parameter in electron pockets the one in 4.7a. We believe it should be possible to find other solutions, based on combinations of these two. For example, we could find a solution in which one of the orbitals in the iron-pnictide follows a behaviour similar to Solution 1 and the other orbital follows the behaviour of Solution 2. However, at this point, we have used several different initial conditions from which to start the iteration and we have not found yet neither an energy-flux relation with local minima at half integer flux quantum values, nor a different spatial phase dependence on flux to those shown in 4.7

We have also probed the parameter space trying to find the “double minimum” regime.

Since this regime can only be caused by the sign changes in the order parameter, it must be found in the regions of parameter space where we the pairs that are tunnelling through the junction are both electron-like and hole-like. We have tested different values of the chemical potential, specially in the s -wave superconductor, in order to make sure that we are on a regime where we find tunnelling from pairs with different order parameter. We have also tried to find the “double minimum” regime by making the hopping amplitudes in the two junctions different. According to Chen *et al.*, the frequency half integer flux quantum transitions measured in their experiment [1] increased when increasing the contact strength across the two superconductors. For this reason, we believe we have only probed relatively high values of the junction’s hopping parameters. Furthermore, since we are interested in describing an $s_{\pm}$, we have kept the values of J_1 and J_2 in the regions of phase space where the $s_{x^2y^2}$ pairing symmetry is dominant. At this point, we have not yet found the “double minimum” regime within the microscopic model. Nevertheless, due to the fact that the solutions found through the iterative method depend strongly on the initial conditions from which we start the iteration, this results are inconclusive.

4.3 Future work

We will discuss mainly two themes in this section: 1) how we plan to find the “double minimum” regime and 2) other phenomena we are interested in analysing within the formalism we have developed.

First, in order to find the “double minimum” regime, we will continue to probe the parameter space in this model. Since there are many different parameters in our model and the self consistency equations have also more than one solution, we need to know where to look for. We could also, in principle, numerically minimize the energy of the system as a function of the order parameter. However, most numerical minimization methods also

rely in an initial guess, and are not guaranteed to find a global minimum. Another option would be to minimize the energy through brute force minimization, but since we have many variables, we do not have the computing resources needed to do this in a reasonable amount of time. Hence, we need to analyse the model carefully, to find an adequate set of parameters and initial conditions in which we could find the behaviour that interests us.

To find an adequate set of parameters and initial conditions, we must start by trying to make a connection with the Ginzburg-Landau type model since it exhibits the energy-flux relation we want to find. In the Ginzburg-Landau type model, when the magnitude of the order parameter is the same for electron and holes, the system was only either in the “time symmetry breaking” regime or in the “double minimum” regime. Therefore, we should be able to easily find the “double minimum” regime if we make the order parameter in electron and hole pockets identical. In order to do this, we need to modify our band structure, the chemical potential, and work in a lattice with the same number of ions in the x and y directions. Something else we could do is to simplify the system by disconnecting one of the junctions. In this case, the phase would no longer need to be periodic in space, which would give the system more freedom, and would allow us to find solutions different to Solution 1 and Solution 2 in the previous section.

Setting the question of finding the “double minimum” regime aside, there are several other phenomena we are interested in studying within our microscopic lattice model. First of all, we are interested in studying the temperature dependence of the system. We would also like to study the behaviour of vortices in this model. Due to the energy periodicity with flux, we have so far focused only on the 0 to Φ_0 interval; however it would also be interesting to analyse the spatial dependence of the solution for larger values of flux. Finally, we could also use the formalism that we have developed to study an iron-pnictide/iron-pnictide composite loop and more complex arrangements, such as, an iron-pnictide/iron-pnictide/ s -wave loop, or an iron-pnictide/ s -wave/ s -wave loop.

Conclusions

Understanding the nature of the pairing mechanism in iron based superconductors is the most fundamental question regarding these materials. Currently, the favourite candidate for this mechanism is magnetic interactions. The nature of magnetic interactions in iron based superconductors is complex, since they do not fit in either the weak or the strong coupling limit. However, theoretical models in both limits predict the same order parameter structure: an $s_{\pm}$ order parameter, which changes signs between the electron and hole Fermi pockets. Obtaining the experimental determination of the pairing symmetry of iron based superconductors would be a first step into determining the pairing mechanism. Since designing and performing phase sensitive experiments that are capable of distinguishing between s -wave and $s_{\pm}$ symmetry, the pairing symmetry of iron based superconductors remains undetermined.

One of the experiments that provides evidence for an unconventional order parameter in iron based superconductors is the phase sensitive experiment performed by Chen *et al.* [1]. In this experiment, Chen *et al.* excited a composite loop made of Niobium and $\text{NdFeAsO}_{0.88}\text{F}_{0.12}$ with electromagnetic pulses, and afterwards measured the relaxation of the pulse as a function of time. With this arrangement they were able to measure both integer and half-integer flux quantum transitions in the loop. Although these results are

clearly incompatible with an s -wave pairing symmetry, it is unclear how they relate to the proposed $s_{\pm}$ symmetry.

In this work, inspired by the phase sensitive experiment performed by Chen *et al.*, we have introduced a microscopic model to study an iron-pnictide/ s -wave composite loop. We believe that we can explain the results of the experiment, through finding an unusual energy-flux relation, with local minima at half integer flux quantum values. Using our microscopic model, we have compared the behaviour of the iron-pnictide/ s -wave composite loop to an s -wave/ s -wave composite loop finding clear differences in the spatial behaviour of the order parameter's phase. Nonetheless, we have not yet found a manifestation of these differences in the energy-flux relation.

We have encountered several numerical difficulties in solving our microscopic model which make our results inconclusive at this point. However, we have already set the formalism necessary to study the iron-pnictide/ s -wave loop. It remains part of our future work to find points of parameter space in which the differences between the two composite loops studied in this work manifest in the energy-flux relation, or to find another measurable property of the system in which these differences manifest.

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