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**A gauge approach to superfluid density  
in high- $T_c$  cuprates**

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# Chapter 1

## Introduction

The high temperature superconductivity (from now on HTSC), is a resistanceless electric current flow observed chiefly in a class of crystals called “cuprates” at very high temperatures compared to those of standard BCS superconductors, so that many of them exhibit superconductivity at temperatures accessible by non-highly-specialized laboratories. To date, the HTSC cuprate with the highest critical temperature is  $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$  which exhibits the superconductive transition at  $135\text{ }^\circ\text{K}$ <sup>1</sup>, see [1].

Starting from its initial experimental observation by Bednorz and Müller in 1986 [2], HTSC has been and still is a major unsolved problem in Theoretical Physics; as soon as it was clear that the BCS theory, which correctly explains superconductivity in a wide range of materials, is not able to successfully describe what happens in a cuprate (see for instance [3]), the research in the HTSC field rapidly developed into many different directions. For an exhaustive review the reader can refer to [3], again. In spite of the huge number of theories which have been proposed in order to explain the phenomenon in the span of nearly two-and-half decades, no fully satisfying theoretical interpretation is known to date. On the other hand, a plethora of

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<sup>1</sup>Some research groups claimed the discovery of material with higher  $T_c$ , but those claims have not (yet) been verified independently.

experimental data is available, making HTSC one of the most experimentally studied physical phenomena in Condensed Matter Physics.

Among the many theories which have been developed in order to explain the HTSC in cuprates, from the very first years an approach pursued by many theorists has been the “spin-charge separation”, pioneered by P.W. Anderson ([4]). According to this viewpoint the fundamental excitations in a HTSC are not simply electron/holes but are spinons and holons, i.e. particles which respectively carry only spin or only charge. This approach in latest years has found support in experimental data which seem to indirectly confirm its correctness, or to confirm it in one-dimensional systems (see for instance [5] and [6]).

Once one agrees that the HTSC can be correctly described in terms of holons and spinons, various choices can be made about how to separate the electron/holes degrees of freedom. Historically two straightforward approaches, called slave fermion and slave boson, have been pursued; more recently a more general and flexible approach has been proposed, an approach which is based upon the Chern-Simons bosonization. Within this framework we can re-obtain the slave boson and slave fermion as particular cases, while introducing at the same time two gauge fields which can be used to correctly describe the symmetries of the system and to catch the essential features of the dynamics of the spinons and of the holons, which ultimately lead to the superconductive transition. In particular one of the Chern-Simons gauge fields takes into account the  $U(1)$  gauge symmetry, while the other one takes into account the  $SU(2)$  spin rotational symmetry of the t-J model, and naturally describes the spinon vortices which play a key role in the onset of the superconductivity. The full superconductivity is then achieved in three steps (condensations of holons, condensation of spinons, coherence) and is mediated by another gauge field which naturally arises from the spin-charge separation.

The topic of the present thesis is the study of superfluid density within such a framework, as proposed in [7]. The superfluid density is a key quantity in a super system, as on one side is one of the most straightforward macroscopically-defined physical observables, while being on the other side intimately correlated with the microscopical behaviour of the superconductor.

In the introductory chapters the superfluid density will be reviewed, both from an historical and experimental point of view; particular attention will be awarded to the various non-equivalent definitions of superfluid density which are commonly used in scientific literature. After an in-depth explanation of the relevant part of the model in [7], finally the calculation of the superfluid density as a function of the temperature, which represents the original contribution of this thesis, will be carried out. The results will be compared with experimental data. An explanation of the physical meaning of the features of the superfluid density just found will be given in the final chapter.





## Chapter 2

# The superfluid density

### 2.1 The superfluid density:

#### a historical perspective and general properties

The superfluid density (in symbols  $\rho_s$ ) is a key quantity in the study and in the description of a superfluid or superconducting system; historically it has represented one of the first, if not the first quantity used in the study of those systems. Following Landau and Lifshitz ([8], § 44) one can give an elementary phenomenological definition of superfluid density in a superconductor, using the so-called “two fluid” phenomenological model. Before briefly introducing this model, it is worth pointing out that as the experimental discovery of SC preceded its microscopical interpretation by more than four decades, for a very long time, for the lack of a better theory, the SC has been analyzed on sheerly phenomenological grounds. Hence the importance of such theories.

The “two fluid” model takes into account two kinds of charge carriers inside a SC: the “normal” electrons, which are subject to resistance, and the “super” charge carriers, upon which no further assumptions are made, except for the fact that they can move without any dissipation; after having made such a simple assumption one can use the standard electrodynamics theory to see the consequences of a resistance-less current flow. Despite its

simplicity, this theory is able to describe many experimental features of a SC, without taking into account the microscopical details and without even knowing which are the charge carriers.

According to this picture, the superfluid density  $\rho_s$  can then be defined as the number density of charge carriers of the second type. Nonetheless one can work a little within this framework and relate  $\rho_s$  with other quantities of the SC system. To do so one notes that as a consequence of the basic assumption of the “two fluids” approach the total current density can be decomposed, when the temperature is in the range  $0 < T \leq T_c$ , as follows:

$$\mathbf{j} = \mathbf{j}_n + \mathbf{j}_s$$

where again  $\mathbf{j}_n$  is a “normal” current density, which is subject to resistance and dissipation by Joule heating, and  $\mathbf{j}_s$  a “super”, dissipation-free current density. Without losing the generality of this treatment, one can describe the probability of finding a super charge carrier in a given position at a given time as the squared modulus of a condensate wave function: denoting with  $\Delta_c(t, \mathbf{r}) \equiv |\Delta_c| e^{i\Phi}$  this wave function, recalling that for a generic wave function in real space representation:

$$\mathbf{v} = \frac{\hbar}{m} \nabla \Phi \quad (2.1)$$

the superfluid density can be implicitly defined by the following relation:

$$\mathbf{j}_s = \rho_s \mathbf{v}_s = \rho_s \frac{e\hbar}{2m_e} \nabla \Phi$$

where  $m_e$  and  $e$  are respectively the mass and the charge of the electron<sup>1</sup>. Here  $\rho_s$ , which is the number density of superconducting electrons and plays

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<sup>1</sup>Here we are forced to take into account the actual microscopical structure of the charge carriers. The factor 2 appears before the electron charge, which is assumed to be negative, because the super charge carriers in a superconductors are pairs of electron, the Cooper pairs.

the very same role of the superfluid fraction in a fluid, is expressed in terms of dynamic variables of the system, as are the current flow and the phase of the condensate wave function. Usually  $\rho_s$  is plotted and studied as a function of temperature.

It is clear that such a description is deeply entailed with a phenomenological description of the superconducting sample, and it is not well suited to be applied where the microscopical details of a superconductor come into play. We will proceed analyzing the consequences of the Landau theory before giving in subsequent sections two more modern definitions of  $\rho_s$  which will be used for the actual calculations throughout the present thesis.

## 2.2 The London equations

The main success of the “two fluid” approach is its success in allowing to derive the London equations which in turn account for one of the key experimentally observed features shared by types of superconductors: the perfect diamagnetism, i.e. the impossibility for a magnetic field to penetrate inside a superconductor. This property, which is also called Meissner effect, is conveniently described in terms of the London penetration depth  $\lambda$ .  $\lambda$  can be, in turn, easily related to the superfluid density. This relation will be used when comparing theoretical results with experimental data.

To derive<sup>2</sup> the London equations one starts roughly from the same hypotheses of the two fluid approach: no knowledge of the structure of the charge carriers is needed. The Newton’s law for a charge inside a superconductor, in the presence of an electric field, reads:

$$m \frac{d\mathbf{v}_s}{dt} = -e\mathbf{E} \quad (2.2)$$

denoting with  $e$  the charge of the SC charge carriers and with  $\mathbf{E}$  the

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<sup>2</sup>Our derivation roughly follows the one in [9].

electric field. As the SC current density can be written as  $\mathbf{j}_s = -e\rho_s\mathbf{v}_s$ , this equation along with eq. 2.2 implies that:

$$\frac{d}{dt}\mathbf{j}_s = \frac{\rho_s e^2}{m}\mathbf{E} \quad (2.3)$$

where  $m$  is the mass of the charge carriers (for a BCS Cooper pair, composed of two electrons, one has  $m = 2m_e$ ). Now one can take the curl of eq. 2.3, and by using Faraday's law of induction  $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$  can obtain:

$$\frac{\partial}{\partial t} \left( \nabla \times \mathbf{j}_s + \frac{\rho_s e^2}{m}\mathbf{B} \right) = 0 \quad (2.4)$$

which, along with Maxwell's equation  $\nabla \times \mathbf{B} = \mu_0\mathbf{j}_s$ , the continuity equation  $\nabla \cdot \mathbf{j}_s = \frac{\partial \rho}{\partial t}$  and the boundary conditions completely determines the magnetic field and the current density inside a superconductor.

It is to be noted that this equation fails at explaining the perfect diamagnetism experimentally observed in an SC, as every time-independent  $\mathbf{B}$  is allowed to arbitrarily penetrate into the insides of the SC material, generating a current density  $\mathbf{j}_s$ , which will be in turn time-independent.

On sheerly phenomenological grounds, to be able to reproduce the Meissner effect, the London brothers modified equation 2.4 into the following, more restrictive, condition:

$$\nabla \times \mathbf{j}_s + \frac{\rho_s e^2}{m}\mathbf{B} = 0 \quad (2.5)$$

This equation, using the Maxwell equations once more<sup>3</sup>, can be rewritten as:

$$\nabla^2 \mathbf{B} = \frac{4\pi\rho_s e^2}{mc^2}\mathbf{B} \quad (2.6)$$

whose solutions can be written in the following form:

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<sup>3</sup>More precisely Ampère's circuital law  $\nabla \times \mathbf{B} = \mu_0\mathbf{j}$  when the fields are time-independent, then the vector calculus identity  $\nabla \times (\nabla \times \mathbf{B}) = \nabla(\nabla \cdot \mathbf{B}) - \nabla^2\mathbf{B}$ , and then  $\nabla \cdot \mathbf{B} = 0$ .

$$B_{\perp}(x) = B_0 \exp\left(-\frac{x}{\lambda}\right) \quad \lambda = \sqrt{\frac{mc^2}{4\pi\rho_s e^2}} \quad (2.7)$$

$B_{\perp}$  being the perpendicular component of the magnetic field, with respect to the surface of the sample, and  $B_0$  being its value at the surface. Equation 2.7 means that while flowing inside a SC a magnetic field decays exponentially, with  $\lambda$  being the length at which it is reduced by a factor  $\frac{1}{e}$ . This parameter is customarily called **London's penetration depth**. It is very important noting for what follows that  $\lambda$  and  $\rho_s$  are correlated by a simple relation:

$$\rho_s \propto \lambda^{-2} \quad (2.8)$$

as  $\lambda$  is a quantity which is quite easily measured experimentally.

## 2.3 Why studying the superfluid density?

As briefly noted in the introduction, there are many reasons for which it is worth studying the superfluid density when testing the validity of newly proposed mechanism for HTSC:

- **Comparability with experiments:** the  $\rho_s$  is one of the fundamental quantities of a superconducting system, and one of the most easily accessible through experiments; for instance the condensate density, being defined on microscopical grounds, is much more difficult to be measured experimentally. Moreover,  $\rho_s$  is related through the simple relation in eq. 2.8 to the London penetration depth  $\lambda$ , which is even more studied from an experimental point of view.
- **Discriminating power between BCS and non-BCS SC:** the superfluid density seems to be a good parameter to tell apart BCS and non-BCS behaviour: in particular, it has been experimentally observed

that cuprates have a much lower  $\rho_s$ , a completely different approach to the critical temperature and will have a very linear  $\rho_s(T)$  behavior for a wide range of temperatures between 0 and an intermediate temperature.

- **Comparability with empirical laws:** the great deal of experimental data available has led to the formulation of various empirical relations for the superfluid density, the most important being the Uemura relation. A new theoretical model must reproduce those empirical results, and, ideally, even try to find a more profound explanation for them.

## 2.4 “Mechanical” definition for $\rho_s$

As previously mentioned, and as discussed in [10], even in scientific literature there is no general agreement over the exact definition of superfluid density; as a result two non-equivalent definitions are commonly employed. In the present and in the following sections those two definitions will be analyzed, along with their phenomenological implications.

The superfluid density can be defined (following [11], [12], [13]) starting from the phase stiffness of the SC condensate wave function phase, i.e. as the energetic cost of slowly and infinitesimally varying the condensate wave function phase. Let us consider the following infinitesimal twist applied to of the condensate wave function (for  $|\mathbf{Q}| \ll 1$ ):

$$\Delta(\mathbf{x}) \longrightarrow \Delta(\mathbf{x}) e^{i\mathbf{Q}\cdot\mathbf{x}} \quad (2.9)$$

it is now easily seen, switching to momentum-space representation, that such a twist is tantamount to imposing an arbitrary extra velocity  $\frac{\mathbf{Q}}{M}$  to each Cooper pair, in a BCS-like theory, or, more generally, to each “super” charge carrier<sup>4</sup>.

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<sup>4</sup>M is the mass of each Cooper pair (so that  $M = 2m_e$ ) or the mass of a generic charge

$$\tilde{\Delta}(\mathbf{p}) = \int d^3x e^{i\mathbf{p}\cdot\mathbf{x}} \Delta(\mathbf{x}) \quad (2.10)$$

$$\implies \int d^3x e^{i\mathbf{p}\cdot\mathbf{x}} \Delta(\mathbf{x}) e^{i\mathbf{Q}\cdot\mathbf{x}} = \int d^3x e^{i(\mathbf{p}+\mathbf{Q})\cdot\mathbf{x}} \Delta(\mathbf{x}) = \tilde{\Delta}(\mathbf{p} + \mathbf{Q}) \quad (2.11)$$

Denoting with  $F(\mathbf{Q})$  the free energy  $F = -\frac{1}{\beta} \ln Z$  of the system when an infinitesimal twist as in eq. 2.9 is applied to the condensate wave function, one can evaluate the free energy difference for small values of  $|\mathbf{Q}|$  and write the first two Taylor expansion terms<sup>5</sup>:

$$\Delta F \equiv F(\mathbf{Q}) - F(0) = |\mathbf{Q}| \left. \frac{\partial F(\mathbf{Q})}{\partial Q} \right|_{|\mathbf{Q}| \rightarrow 0} + \frac{|\mathbf{Q}|^2}{2} \left. \frac{\partial^2 F(\mathbf{Q})}{\partial Q^2} \right|_{|\mathbf{Q}| \rightarrow 0} + O(|\mathbf{Q}|^3) \quad (2.12)$$

As seen in eq. 2.10 and 2.11 when imposing the infinitesimal twist, from a physical point of view one is simply shifting the speed of the Cooper pairs as described in the following way:

$$\mathbf{v} \longrightarrow \mathbf{v}' = \mathbf{v} + \frac{\hbar}{M} \mathbf{Q}$$

so that the free energy variation will take account for the extra kinetic energy, being then proportional to  $|\frac{\hbar}{M} \mathbf{Q}|^2$  and so quadratic in  $|\mathbf{Q}|$ . One is then allowed to take eq. 2.12 and discard all terms but the second when Taylor-expanding  $\Delta F$ :

$$\Delta F \equiv F(\mathbf{Q}) - F(0) = \frac{|\mathbf{Q}|^2}{2} \left. \frac{\partial^2 F(\mathbf{Q})}{\partial Q^2} \right|_{|\mathbf{Q}| \rightarrow 0}$$

It is also clear that the twist in eq. 2.9 affects only the superconducting pairs, leaving the non-superconducting fraction of the system untouched, so that the superfluid density can be implicitly defined as follows:

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carrier.

<sup>5</sup>Elementary symmetry considerations show that  $\Delta F$  will be dependent only upon  $|\mathbf{Q}|$  rather than  $\mathbf{Q}$ , justifying the expansion.

$$\Delta F = \frac{1}{2}\rho_s m v_s^2 \implies \rho_s \equiv 4m \left. \frac{\partial^2 F(\mathbf{Q})}{\partial Q^2} \right|_{|\mathbf{Q}| \rightarrow 0} \quad (2.13)$$

To have a different insight upon the definition we just gave, one can also think of eq. 2.13 as a measure of the phase coherence for the condensate wave function of the system. If long-range phase coherence is present in the system, there will be a free energy variation when imposing a position-dependent phase twist to the order parameter. On the contrary, if the phase of the condensate wave function were in a disordered state, changing the phase would not have any energetic cost.

## 2.5 “Electromagnetic” definition for $\rho_s$

Alternatively  $\rho_s$  can also be defined as the coefficient governing phase fluctuations in an effective action for superconductivity:

$$S_{\text{EFF}} = \frac{\rho_s}{2} \int d\tau \int d^d r (\nabla\theta)^2 + (\text{other non quadratical in } \nabla\theta \text{ terms}) \quad (2.14)$$

In what follows we shall derive, following the treatment in [14], such an effective action in the BCS theory framework to see how this definition can be linked to physical observables of a SC system. In order to do so we recall that the BCS Hamiltonian is written as:

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}, \sigma} - \frac{g}{L^d} \sum_{\mathbf{k}, \mathbf{k}', \sigma} c_{\mathbf{k}+\mathbf{q}, \uparrow}^\dagger c_{-\mathbf{k}, \downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q}, \downarrow} c_{\mathbf{k}', \uparrow} \quad (2.15)$$

with the usual notation for the electron creation/annihilation operators and for the number operator,  $g$  being a positive constant. The interaction term in the Hamiltonian allows electrons to scatter from a two-electron state  $|\mathbf{k} \uparrow, -\mathbf{k} \downarrow\rangle$  to a two-electron state  $|\mathbf{k} + \mathbf{q} \uparrow, -\mathbf{k} - \mathbf{q} \downarrow\rangle$  with both the initial and final momentum states being close to the Fermi surface. Even if in a very simplified way, as the coupling  $g$  should in general also depended upon the



transferred momentum, the Hamiltonian in eq. 2.15 can be used to study the celebrated Cooper instability, i.e. the instability of the electron gas towards the formation of Cooper pairs, which are time-reversed two-electron states such as  $|\mathbf{k} \uparrow, -\mathbf{k} \downarrow\rangle$ . Cooper instability appears under a certain finite critical temperature  $T_c$  and only in presence of an attractive interaction between electrons, which can be even extremely feeble; this attraction is provided by the electron-lattice interaction due to the different time scales of electron and phonon propagation, and leads to a finite expectation value of time-reversed pairs such the one discussed above, so that the the order parameter for the BCS can be taken to be:

$$\Delta = \frac{g}{L^d} \sum_{\mathbf{k}} \langle \Omega | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \Omega \rangle$$

The superconductive phase properties can then be derived by studying the theory in an opportune mean-field approximation. As far as the superfluid density is concerned we begin by noting that starting from eq. 2.15 the partition function for the BCS theory, minimally coupled to the electromagnetic field, reads:

$$Z = \int \mathcal{D}(\psi, \bar{\psi}) e^{-S[\psi, \bar{\psi}]}$$

$$S[\psi, \bar{\psi}] = \int_0^\beta d\tau \int d^d r \left[ \bar{\psi}_\sigma \left( \partial_t + ie\phi + \frac{1}{2m} (-i\nabla - e\mathbf{A})^2 - \mu \right) \psi_\sigma - g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\uparrow \psi_\downarrow \right]$$

We note that this theory is invariant for a local  $U(1)$  gauge group of transformations, namely:

$$\begin{aligned} \psi &\longrightarrow e^{i\theta(\tau, \mathbf{x})} \psi & \bar{\psi} &\longrightarrow e^{-i\theta(\tau, \mathbf{x})} \bar{\psi} \\ \phi &\longrightarrow \phi - \frac{\partial_\tau \theta(\tau, \mathbf{x})}{e} & \mathbf{A} &\longrightarrow \mathbf{A} + \frac{\nabla \theta(\tau, \mathbf{x})}{e} \end{aligned} \quad (2.16)$$

Such a theory can be rewritten by using an Hubbard-Stratonovich transformation to decouple the quartic interaction in the Cooper channel. Then, by using the Nambu spinor formalism, the theory can be recast as:

$$\bar{\Psi} = (\bar{\psi}_\uparrow, \psi_\downarrow) \quad \Psi = \begin{pmatrix} \psi_\uparrow \\ \bar{\psi}_\downarrow \end{pmatrix}$$

$$Z = \int \mathcal{D}(\psi, \bar{\psi}) \mathcal{D}(\Delta, \bar{\Delta}) \exp \left( - \int d\tau d^d r \left[ \frac{|\Delta|^2}{g} - \bar{\Psi} \mathcal{G}^{-1} \Psi \right] \right) \quad (2.17)$$

where now  $\Delta$  is redefined as the bosonic field used in the Hubbard-Stratonovich transformation; we note that for the transformation group in eq. 2.16 the  $\Delta$  field transforms as  $\Delta \rightarrow \Delta e^{2i\theta(\tau, \mathbf{x})}$ , and:

$$\mathcal{G}^{-1} = \begin{pmatrix} -\partial_t - ie\phi - \frac{1}{2m} (-i\nabla - e\mathbf{A})^2 + \mu & \Delta \\ \bar{\Delta} & -\partial_t - ie\phi - \frac{1}{2m} (-i\nabla - e\mathbf{A})^2 + \mu \end{pmatrix}$$

In eq. 2.17 one can carry out the functional integration over the fermionic variables  $\psi$  e  $\bar{\psi}$  obtaining:

$$Z = \int \mathcal{D}(\Delta, \bar{\Delta}) \exp \left( - \frac{1}{g} \int d\tau d^d r |\Delta|^2 + \ln \det \mathcal{G}^{-1} \right)$$

By definition  $\Delta$  counts the number of Cooper pairs, so that it can be used as order parameter for the superconducting transition: above  $T_c$  one sees that  $|\Delta| = 0$  and the phase remains undefined; on the other hand below  $T_c$  a fundamental state with a fixed phase is created and equivalent fundamental states are connected by a phase rotation of the order parameter  $\Delta \rightarrow \Delta e^{i\theta}$ . In other words the superconductive transition in the BCS theory corresponds to a  $U(1)$  local symmetry breaking.

The effective action in eq. 2.14 corresponds exactly to an effective action for the Goldstone mode for  $T \leq T_c$ ; by following, again, [14] such an effective action can be written down starting from simple physical arguments and assumptions on the symmetry of the system. Specifically, an effective action for the Goldstone mode for the BCS theory must respect the following constraints:

- All the terms should go to zero in the  $\theta \rightarrow \text{constant}$  limit.
- The gradients and the temporal derivatives of  $\theta$  must be sufficiently slow-varying so that a first-order Taylor-series expansion is justified.
- Due to the symmetries of the system the effective action cannot contain neither terms with an odd number of derivatives, nor terms with mixed temporal/spatial derivatives.
- The resulting action must have the same symmetries of the original BCS theory, particularly it must be invariant for the transformations in eq. 2.16.

The most general form for an effective action respecting all the aforementioned constraints is:

$$S[\theta] = \int d\tau d^d r \left[ c_1 (\partial_\tau \theta)^2 + c_2 (\nabla \theta)^2 \right]$$

For consistency with the original action we can then couple the electromagnetic field, by minimal substitution, also adding a kinetic term for the electromagnetic field:

$$S[\theta, \mathbf{A}] = \int d\tau d^d r \left[ c_1 (\partial_\tau \theta + \phi)^2 + c_2 (\nabla \theta - \mathbf{A})^2 \right] + \frac{1}{4} \int d\tau d^d r F_{\mu\nu} F^{\mu\nu} \quad (2.18)$$

Assuming of describing the system at a high enough temperature  $0 < T \leq T_c$  so that the quantum fluctuation can be neglected (i.e.  $\partial_\tau \phi = 0$ ) and also assuming that there are no electric fields inside the superconductor, (i.e.  $\phi = 0$  e  $\partial_\tau \mathbf{A} = 0$ ) then eq. 2.18 simplifies to:

$$S[\theta, \mathbf{A}] = \frac{\beta}{2} \int d^d r \left[ \frac{\rho_s}{m} (\nabla \theta - \mathbf{A})^2 + (\nabla \times \mathbf{A})^2 \right]$$

where  $c_2$  has been redefined in terms of  $\rho_s$ . The gaussian integral over the  $\theta$  variable can be carried out, as  $\theta$  appears quadratically in the action; in

order to do so it is convenient rewriting the action as a sum in momentum space<sup>6</sup>:

$$S[\mathbf{A}] = \frac{\beta}{2} \sum_{\mathbf{q}} \left( \frac{\rho_s}{m} \left( \mathbf{A}_{\mathbf{q}} \cdot \mathbf{A}_{-\mathbf{q}} - \frac{(\mathbf{q} \cdot \mathbf{A}_{\mathbf{q}})(\mathbf{q} \cdot \mathbf{A}_{-\mathbf{q}})}{q^2} \right) + (\mathbf{q} \times \mathbf{A}_{\mathbf{q}}) \cdot (\mathbf{q} \times \mathbf{A}_{-\mathbf{q}}) \right) \quad (2.19)$$

This action can be rewritten in a simpler way by separating the longitudinal and transverse components of  $\mathbf{A}_{\mathbf{q}}$  as follows:

$$\mathbf{A}_{\mathbf{q}} = \underbrace{\mathbf{A}_{\mathbf{q}} - \frac{\mathbf{q}(\mathbf{q} \cdot \mathbf{A}_{\mathbf{q}})}{q^2}}_{\equiv \mathbf{A}_{\mathbf{q}}^{\perp}} + \underbrace{\frac{\mathbf{q}(\mathbf{q} \cdot \mathbf{A}_{\mathbf{q}})}{q^2}}_{\equiv \mathbf{A}_{\mathbf{q}}^{\parallel}}$$

substituting in the action in eq. 2.19:

$$S[\mathbf{A}] = \frac{\beta}{2} \sum_{\mathbf{q}} \left( \frac{\rho_s}{m} + q^2 \right) \mathbf{A}_{\mathbf{q}}^{\perp} \mathbf{A}_{-\mathbf{q}}^{\perp} \quad (2.20)$$

This is the Anderson-Higgs mechanism in action; when the Goldstone mode  $\theta$  is integrated out then electromagnetic field acquires a mass term, namely  $\frac{\rho_s}{m}$ ; from this action it is also immediate deriving the equations of motion for the transverse component of  $\mathbf{A}$ :

$$\left( \frac{\rho_s}{m} - \nabla^2 \right) \mathbf{A}^{\perp}(\mathbf{r}) = 0$$

from which, by taking the curl of both sides, the first London equation can be derived:

$$\left( \frac{\rho_s}{m} - \nabla^2 \right) \mathbf{B}^{\perp}(\mathbf{r}) = 0 \quad (2.21)$$

When  $\rho_s \neq 0$ , eq. 2.21 has only exponentially decaying solutions, i.e.  $\mathbf{B}^{\perp} \propto \exp\left(-\frac{x}{\lambda}\right)$  so that the transverse component of the magnetic field,

<sup>6</sup>We only give the final result, for a complete derivation the reader is referred to [14]

when penetrating a superconductor is exponentially suppressed with a characteristic decay length  $\lambda \propto \sqrt{\frac{m}{\rho_s}}$ , which is in perfect accordance with eq. 2.7. The decay length is, generally, much shorter than the dimensions of superconductive samples used by experimentalists, so that commonly it is said that a SC ejects magnetic fields from its inside by means of Meissner effect.

As previously seen London equations have been derived long before the advent of BCS theory and can be derived on sheerly phenomenological grounds, assuming that only part of the electrons is participating in the resistance-less current flow, its numerical density being  $\rho_s$ :

$$\mathbf{j}_s = -\rho_s e \mathbf{v}_s$$

By retracing the steps in the present section which lead us from the BCS theory to London equation it is easily seen how the coefficient governing phase fluctuations, as described at the very beginning of this section, is indeed the superfluid density.

## 2.6 $\rho_s^{\text{F}}$ vs. $\rho_s^{\text{EM}}$

From the definitions given in the previous section it is clear that the mechanically-defined superfluid density (from now on  $\rho_s^{\text{F}}$ ) and the electromagnetically-defined superfluid density (from now on  $\rho_s^{\text{EM}}$ ) are in general *not* the same quantity. An exhaustive contrastive review of  $\rho_s^{\text{F}}$  and  $\rho_s^{\text{EM}}$  can be found in [10], along with a derivation of the following relation between these two quantities:

$$\rho_s^{\text{F}} = \rho_s^{\text{EM}} \left( 1 - \frac{4\pi^2 \rho_s^{\text{EM}} L^{d-2}}{T} \langle I^2 \rangle \right) \quad (2.22)$$

the average over  $I^2$  being taken with the following un-normalized distribution:

$$W_I \propto e^{-\frac{2\pi^2 \rho_s^{\text{EM}} L^{d-2}}{T}} I^2$$

For the aim of the present thesis, it is important noting that:

- Equation 2.22 obviously holds only when both quantities are defined; particularly  $\rho_s^{\text{EM}}$  may be undefined as  $\nabla\theta$  need to be a well-defined function.
- By looking at eq. 2.20 one can understand that  $\rho_s^{\text{EM}}$  is indeed the quantity associated with the spontaneous symmetry breaking and with the gauge field acquiring a mass gap due to the Anderson-Higgs mechanism;  $\rho_s^{\text{EM}}$  is deeply entailed with the microscopical mechanisms of SC.
- On the other hand one may say that  $\rho_s^{\text{F}}$  is only incidentally related to  $\rho_s^{\text{EM}}$  in the BCS theory: it is not related to the gauge field becoming gapped, but to the formation of a finite density of incoherent electron pairs, as clear when referring to section 2.4. As the electron pairs condense and become coherent at the same time in the BCS theory framework, this difference is not observable and the two definitions are effectively interchangeable. However, when dealing with more sophisticated theories with two different temperatures for pair condensation and coherence this difference must be taken into account.
- As noted in [10] for sheerly numerical reasons in three-dimensional systems  $\rho_s^{\text{F}} \approx \rho_s^{\text{EM}}$  up to a part in  $10^4$ , so that even in this case the two definitions are interchangeable.

Throughout the present thesis we will refer, as commonly done in scientific literature, to a generic superfluid density  $\rho_s$ , emphasizing the difference between the two definitions only when essential to the discussion.

We also note that usually in experimental reports of superfluid density usually one is dealing with  $\rho_s^{\text{EM}}$ . Usually  $\rho_s^{\text{EM}}$  is calculated from  $\lambda$ , which in turn is measured directly or with muon spin relaxation ( $\mu\text{SR}$ ) techniques. Even if it would be possible in principle to directly measure  $\rho_s^{\text{F}}$  with a torsional oscillator, no such experiment is known to the author at the time of writing.

## 2.7 Theoretical predictions and experimental data for superfluid density

From a theoretical point of view, following [15] and citations therein, one can obtain an analytical expression for the superfluid density within a two-fluid model and within the BCS theory. In the aforementioned paper one can find that the analytical dependence of the penetration depth as a function of temperature reads as follows:

$$\begin{cases} \lambda(T) = \frac{\lambda(T=0)}{\sqrt{1-\left(\frac{T}{T_c}\right)^4}} & \text{(two-fluid model)} \\ \lambda(T) = \frac{\lambda(T=0)}{\sqrt{1-\left(\frac{T}{T_c}\right)^{3-\left(\frac{T}{T_c}\right)}}} & \text{(BCS theory)} \end{cases}$$

which in turn readily yields, through eq. 2.8, an expression for the superfluid density (to be more precise we are now dealing with  $\rho_s^{\text{EM}}$ ):

$$\begin{cases} \rho_s(T) = \rho_s(T=0) \left[ 1 - \left(\frac{T}{T_c}\right)^4 \right] & \text{(two-fluid model)} \\ \rho_s(T) = \rho_s(T=0) \left[ 1 - \left(\frac{T}{T_c}\right)^{3-\left(\frac{T}{T_c}\right)} \right] & \text{(BCS theory)} \end{cases} \quad (2.23)$$

Equations 2.23 are plotted in fig. 2.1, the main difference between the two cases being the approach to the critical temperature which is:

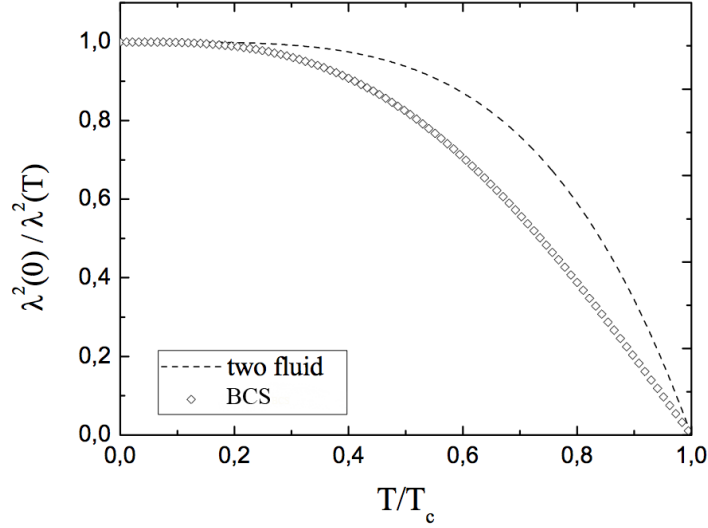


Figure 2.1:  $\rho_s$  as a function of temperature, as predicted by the “two fluid” model and by standard BCS theory, taken from [15]

$$\begin{cases} \rho_s(T) \underset{T \rightarrow T_c}{\sim} 4t & \text{(two-fluid model)} \\ \rho_s(T) \underset{T \rightarrow T_c}{\sim} 2t & \text{(BCS theory)} \end{cases}$$

having introduced the adimensional quantity  $t \equiv \frac{T_c - T}{T_c}$ . The “two-fluid model” agrees with the microscopical theory as long as the global behaviour of the superfluid density is concerned, but fails at catching the actual details of the superconductive transition at  $T = T_c$ .

Obviously there is no analytical formula for the temperature dependence of  $\rho_s$  in cuprates; however this parameter, along with the London penetration depth to which it is correlated, has been widely investigated experimentally. Fig. 2.2, shows that  $\rho_s$  in cuprates diverges appreciably from BCS theory: the key differences can be seen as  $T \rightarrow 0$  and at  $T = T_c$ :

- At zero temperature both the BCS theory and the two fluid model predict that for  $T \rightarrow 0$  the first derivative with respect to temperature



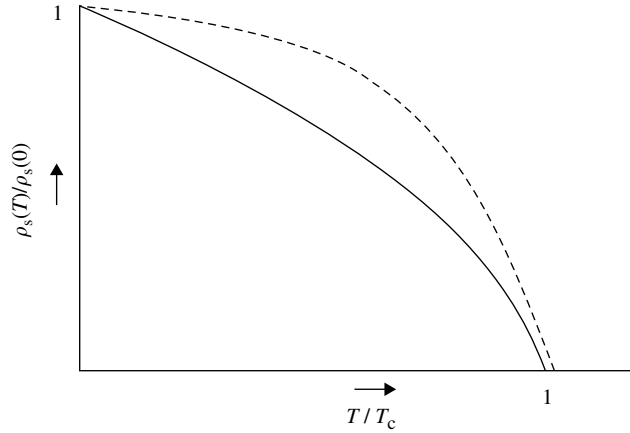


Figure 2.2: Superfluid density as a function of temperature, as measured from the London penetration depth, in a BCS superconductor (dashed line) and in a cuprate superconductor (solid line). The  $x$  and  $y$  axes are rescaled to make  $T_c$  and  $\rho_s(T=0)$  coincide. Taken from [3]

of  $\rho_s$  should go to zero as well, as can be easily derived from eq. 2.23. On the contrary, experimental data shows that for HTSC cuprates  $\left. \frac{d\rho_s}{dT} \right|_{T=0} \neq 0$ . Furthermore the linearity of  $\rho_s$  can extend to quite high temperature, as high as  $\frac{T_c}{2}$ . Usually this behaviour is parametrized as follows:

$$\rho_s \sim 1 - \alpha T \quad \text{for } T \rightarrow 0 \quad (2.24)$$

- The critical temperature approach is quite peculiar to cuprates: it has been noted that, in the vicinity of the critical temperature, the critical exponents seems to be the one of a 3D XY model. This implies that  $\rho_s$  can be parametrized as follows:

$$\rho_s \sim \left| \frac{T - T_c}{T_c} \right|^\delta \quad \text{for } T \rightarrow T_c \quad (2.25)$$

with  $\delta \approx 0.66$ .

Experimentally those two features of cuprates have been extensively verified for a wide variety of cuprate compounds:

- The linearity of the superfluid density in proximity of the absolute zero has been verified both directly and indirectly, i.e. by verifying the linearity of  $\lambda$  as in  $\lambda(T) = 1 + \beta T$ , which in turn implies linearity for  $\rho_s$  as parametrized in eq. 2.24 with  $\alpha = -2\beta$ . More specifically the linearity has been verified for YBCO (see [16]), for BSCCO (see [17] and [18]), for  $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$  (see [19]); the interested reader is referenced to [20] and citations therein for a full experimental review of the topic. In addition to that, as shown in fig. 2.4, the low-temperature behaviour of  $\rho_s$  is also a means of ruling out an s-wave order parameter, further differentiating the cuprates physics from standard superconductors.

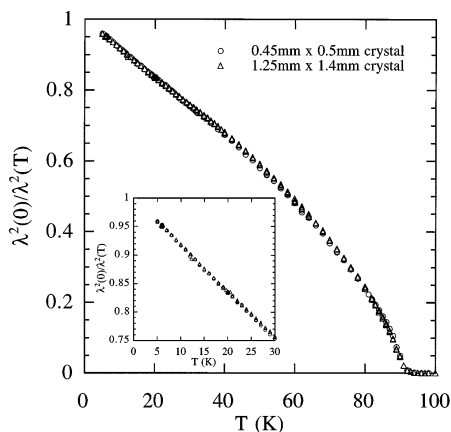


Figure 2.3: Superfluid density for BSCCO, as shown in [17]. The typical features of  $\rho_s$  in cuprates, namely the XY-like transition and the linearity at low  $T$  are evident.

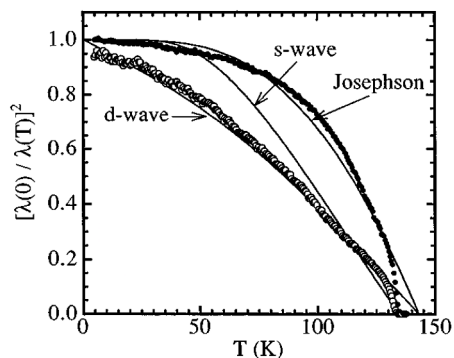


Figure 2.4: taken from [19]. The superfluid density for HBCCO (in open circles) is quite consistent with a d-wave pairing, as opposed to the BCS theory which predicts an s-wave pairing.

- It has been argued by many, starting from shortly after the discovery of

HTSC, that the superconducting transition seems to be in the 3DXY universality class. For instance Kamal et. al ([21]) verified that the penetration depth in YBCO for a range of temperature is consistent with a 3D XY critical behaviour, namely  $\lambda(T) \propto \left| \frac{T-T_c}{T_c} \right|^{-\gamma}$  with  $\gamma \approx 0.33$ , which implies in eq. 2.25  $\delta \approx 0.66$ . An identical behaviour has been observed for BSCCO ([22]) and for optimally-doped LSCO ([23])

Moreover, as observed in [24] the London penetration depth for all cuprates is consistently in the  $0.1\mu\text{m}$  order of magnitude; on the other hand the London penetration depth for superconductors correctly described by the BCS theory is short, in the order of  $0.01\mu\text{m}$ , as noticed in [25] for mono-elemental superconductors. It follows that cuprates show a low superfluid when compared to standard superconductors.

In conclusion of this section, it is worth mentioning an empirical relation which holds for all cuprates, known as **Uemura relation**, according to which the critical temperature of a cuprate depends linearly on the superfluid density at  $T = 0$ , this dependence being universal for all cuprates in the underdoped regime. In formulas:

$$T_c \propto \rho_s(T = 0)$$

Such a correlation in experimental data, discovered by Uemura and coworkers in 1989 is believed to catch fundamental insight about non-conventional superconductivity, as it applies to various classes of non-conventional superconductors (along with cuprates, also bismuthates, organic compounds, heavy-fermion compounds) while not applying to BCS superconductors<sup>7</sup>.

A complete theory of superconductivity in cuprates must explain all those differences between HTSC and BCS theories.

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<sup>7</sup>An extended review of the Uemura relation and its scope of application can be found in [26]



## Chapter 3

# High temperature superconductivity in cuprates

### 3.1 Common features of the cuprates

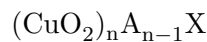
The aim of this chapter is to introduce some basic chemical and physical properties of the HTSC cuprates; this class of material encompasses a great deal of different materials, which share a few key properties, while differing at the same time for many other features. It is then very reasonable to assume that the HTSC arises from the shared features, and that one is allowed, at least in a first approximation, to overlook the details which are specific only to one or few materials.

All of the HTSC cuprates share the following characteristics:

- An HTSC cuprate exhibits superconductivity at temperatures as high as 135 °K, much higher than those of “standard” superconducting materials. The BCS theory can account for the onset of superconductivity only for temperatures as high as 30 °K.
- In these materials the SC cannot be described within the framework of the BCS theory. This claim is supported by many experimental

observations, the most significant being:

- There is no electron-phonon interaction (see for instance [3]); this reason alone would be enough to rule out any BCS-like SC.
  - The order parameter is of  $d_{x^2-y^2}$  type so that it has d-wave symmetry, as opposed to the s-wave symmetry of BCS SC.
- The unit cell of a cuprate is composed of a number  $n$  of  $\text{CuO}_2$  layers (see fig. 3.1<sup>1</sup>), each one of these layers being a square lattice with Cu atoms at each lattice site, and an O atom at midpoint between each lattice site. These layer are separated by  $n - 1$  mono-elemental “spacer” layers. In addition to that, in many but not all cuprates there are also other atoms above and below the aforementioned layers, variously structured, which act as “charge reservoir”. It is customary to orient the crystallographic axes so that the  $\text{CuO}_2$  planes lie in the  $a - b$  plane, with the  $c$  axis perpendicular to those planes. The  $\text{CuO}_2$  planes are widely believed to be the main seat of the superconductivity, while the role of the other structures is debated. The lattice spacing for the copper-oxygen layer is about 3.8 Å, while the length of the unit cell along the c-axis can be as long as 15 Å.
  - As a consequence of the chemical structure of the cuprates, their chemical formula can be written in the following form, as proposed by Leggett in [3]:



where A is an alkaline earth, rare earth, Y, La or a mixture of these elements and X is an arbitrary collection of elements, which may contain other coppers or oxygens. This expression is particularly convenient

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<sup>1</sup>Image by James Slezak, released under Creative Commons BY-SA 3.0 license.

because when one writes a cuprate's chemical formula this way is making its structure, in terms of  $\text{CuO}_2$  planes, "spacer" atoms A and the charge reservoir X, immediately evident.

A few examples:

Common name	Standard chemical formula	n	Notation as proposed by Leggett
BSCCO	$\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$	2	$(\text{CuO}_2)_2\text{CaBi}_2\text{Sr}_2\text{O}_{4+\delta}$
YBCO	$\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$	2	$(\text{CuO}_2)_2\text{YBa}_2\text{CuO}_{2+\delta}$
LSCO	$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$	1	$(\text{CuO}_2)\text{La}_{2-x}\text{Sr}_x\text{O}_2$
HgBCO	$\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$	3	$(\text{CuO}_2)_3\text{Ca}_2\text{HgBa}_2\text{O}_2$
NCCO	$\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$	1	$(\text{CuO}_2)\text{Nd}_{2-x}\text{Ce}_x\text{O}_2$
$\infty$ -layer	$\text{Sr}_x\text{Ca}_{1-x}\text{CuO}_2$	1	$(\text{CuO}_2)\text{Sr}_x\text{Ca}_{1-x}$

- Superconductivity ensues only when the material is doped, i.e. a small amount of impurity is introduced in the form of a small excess or defect of one element, or as a small amount of a different element substituting part of the atoms of an element in the parent compound. As a consequence the stoichiometric formula is now fractionary and contains the doping amount as a parameter, e.g.:



for the material commonly referred to as BSCCO. The doping is fundamental to achieve superconductivity, nonetheless usually superconductivity ensues for small values of the doping, which bring us to an almost perfect stoichiometry. An undoped cuprate is called "parent compound" with respect to the same cuprate, when doped.

- The doping plays, as seen, a key role in the onset of HTSC, but at the same time an equally important role is played by temperature. One

can be more specific by drawing the phase diagram in terms of doping<sup>2</sup> ( $x$  axis) and temperature ( $y$  axis), and will see that is strikingly similar for all the cuprates.

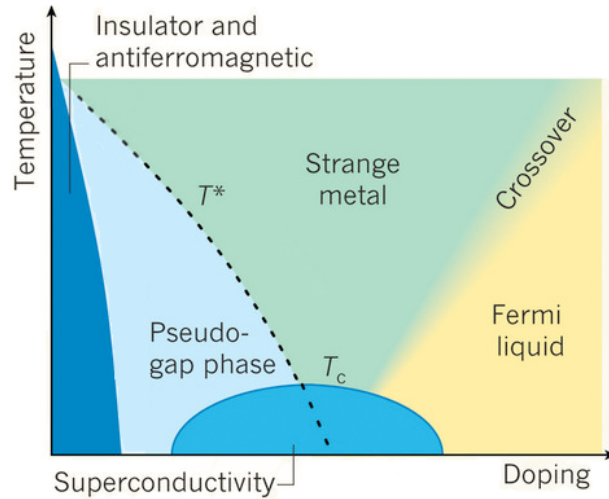


Figure 3.2: The phase diagram, an universal feature for cuprates, from [27]

More specifically, all SC cuprates exhibit in their phase diagram a superconductive dome which starts at  $\delta \approx 0.05$  and ends at  $\delta \approx 0.27$ , centered around the so-called optimal doping at  $x \approx 0.15$ , which is the doping value for which the SC can be achieved at the highest temperature. The superconducting dome is universal in its shape once the  $y$  axis is rescaled so that  $T_c \rightarrow 1$  at optimal doping. The regions with lower and higher doping than the optimal value are respectively called underdoped and overdoped regions. Even outside the superconductive dome, the properties of the cuprates are somewhat strange, and are far from being fully understood:

- For sufficiently low doping<sup>3</sup> and temperatures the system is a Mott

<sup>2</sup>For the phase diagram to be universal one must consider as doping only the holes actually injected into the  $\text{CuO}_2$  planes.

<sup>3</sup>The zero doping condition is also referred as “perfect” stoichiometry.



insulator; the spins are in a staggered (**anti-ferromagnetic**) configuration to minimize the energy.

- The **pseudogap** (PG) regime is characterized mainly by a depletion of states close to the Fermi surface, hence its name. From an experimental point of view the PG regime is characterized by the appearance of a Fermi surface made of four disconnected arcs, as seen in ARPES<sup>4</sup> experiments; these arcs shrink down to just nodal points as the temperature is lowered approaching the superconducting dome. This structure is intermediate between a full Fermi connected surface at higher temperature and the nodal structure in the SC state, and retains the same  $d_{x^2-y^2}$  symmetry of the SC order parameter. The d.c. resistivity, probably the most studied parameter for cuprates, is somewhat strange in the PG regime: it decreases steeply, i.e.  $\rho(T) \propto T^\alpha$  with  $0 < \alpha < 1$  for intermediate temperatures and then diverges for  $T \rightarrow 0$ . A great deal of theories has been postulated in order to explain the strange properties of the PG regime: according to some authors it is a sort of precursor of SC, while according to others the PG regime is to be explained separately.
- The PG and the **strange metal** (SM) regions are separated by what is possibly a phase transition. On the contrary above the underdoped zone of the phase diagram one has the SM and Fermi liquid (FL) regions which are not separated by a transition; indeed one sees that the description of the system diverge more and more abruptly from a standard Fermi liquid description, by lowering the doping, even before undergoing the PG/SM transition. For instance the d.c. resistivity has a behaviour  $\rho(T) \propto T^\alpha$  with  $\alpha$  varying continuously from  $\alpha \sim 2$  in the FL regime to  $\alpha \sim 1$  in the

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<sup>4</sup>Angle-resolved photoemission spectroscopy

SM region near optimal doping. It is interesting noting that for the relation  $\rho(T) \propto T$  near optimal doping the intercept seems to be very close to zero, and also the slope does not vary appreciably between different cuprate compounds.

### 3.2 The $t/J$ model in describing the physics of cuprates

Let us go back to the description of cuprates in terms of  $\text{CuO}_2$  planes, without any doping<sup>5</sup>. Each copper atom, being in the  $2+$  oxidation state has all its orbitals completely filled, apart from the most energetic  $2d(x^2 - y^2)$  orbital which contains one unpaired electron. The oxygen atoms, on the other side, being in the  $2-$  oxidation state have a complete octet and have their  $2p$  shells completely filled. An equivalent description, which is more functional to the aims of the present thesis, can be given in terms of holes: one can equivalently say that at half-filling (i.e. without any doping) there is a hole for each copper site, while, on the other hand, no holes are present on the oxygen atoms.

Moreover, four oxygens around a copper site hybridize their  $p$  orbitals forming an hybrid orbital which has the same symmetry of the central  $3d_{x^2-y^2}$  Cu orbital. When doping is added to the system, some additional holes are introduced. It has been argued ([28]) that these additional holes are shared on the combination of the oxygen  $p$  orbitals. To minimize the energy the spin of this hole is opposite to the spin of the copper atom it surrounds, forming a spin singlet which is called Zhang-Rice singlet.

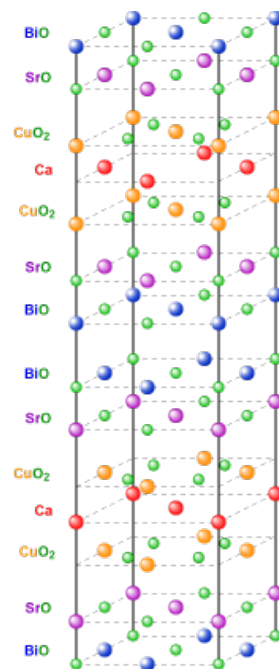


Figure 3.1: The unit cell for BSCCO.

<sup>5</sup>With respect to a doped cuprate, its undoped version is called “parent compound”

Such a structure (four hybridized O orbitals surrounding a hole on a Cu) is believed by many authors to be one of the main features which lead to SC. One should also note that such a structure has an overlap (one oxygen atom) with the very same structure centered on a neighbouring lattice site and introduce a hopping probability for a Zhang-Rice singlet which allows it to move in the anti-ferromagnetic background.

To sum up, if one wants to develop a theoretical model which accounts for the dynamics of the clusters just described, must at least introduce the following features<sup>6</sup>:

- A kinetic term, which takes into account the possibility for a hole to jump to neighbouring site:

$$H_{\text{kinetic}} = -t \sum_{\langle i,j \rangle} \left( \sum_{\alpha} c_{i\alpha}^{\dagger} c_{j\alpha} + h.c. \right)$$

where each  $c_{i,\alpha}$  ( $c_{i,\alpha}^{\dagger}$ ) destroys (creates) a hole on the  $i$  lattice site and  $\alpha$  is a spin index,  $\alpha = \uparrow, \downarrow$

- An anti-ferromagnetic Heisenberg term take into account the fact that the spin momenta of the Cu atoms prefer a staggered configuration in the low-energy limit, the energetic cost to pay for aligning two neighbouring spin being  $J$ :

$$H_{\text{Heisenberg}} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

here  $\mathbf{S}_i \equiv \sum_{\alpha,\beta} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}$  is the spin of the  $i$ -th site.

- Lastly, we need to take into account the strong on-site repulsion on each Cu site: the energy penalty for having two holes residing on the

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<sup>6</sup>For a rigorous demonstration of how the low-energy physics of ZR singlets map to the  $t/J$  model the reader is referred to [28].

same oxygen site is about 10 eV, so that in first approximation one can impose a no-double-occupancy constraint. Such a constraint is thereby imposed by using the Gutzwiller projector:

$$P_G \equiv \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$$

The high non-linearity of  $P_G$  is the main problem which hinders an analytical solution for this category of problems.

In the end one can combine all these features together, obtaining an hamiltonian which describes a model known as  $t/J$  model:

$$H_{t/J} = \sum_{\langle i,j \rangle} P_G \left[ -t \sum_{\alpha} c_{i\alpha}^{\dagger} c_{j\alpha} + h.c. + J \mathbf{S}_i \cdot \mathbf{S}_j \right] P_G \quad (3.1)$$

The physics of this model depend strongly on the ratio  $t/J$ ; from numerical simulations one can see that the typical values for the parameters of the  $t/J$  model in cuprates are:  $t \approx 0.4$  eV and  $J \approx 0.13$  eV. Alternatively the very same model can be implemented in an equivalent way, more suited for path-integral approaches, by writing down an equivalent Euclidean action in terms of spin  $\frac{1}{2}$  Grassmann fermionic fields<sup>7</sup>:

$$S_{t/J} = \int_0^{\beta} d\tau \left\{ \sum_{\langle i,j \rangle} \left( -\frac{J}{2} |\Psi_{i,\alpha}^* \Psi_{j,\alpha}|^2 + [-t (\Psi_{i,\alpha}^* \Psi_{j,\alpha} + h.c.)] \right) + \sum_i \Psi_{i,\alpha}^* (\partial_0 + \delta) \Psi_{i,\alpha} + \sum_{i,j} u_{i,j} \Psi_{i,\alpha}^* \Psi_{j,\beta}^* \Psi_{j,\beta} \Psi_{i,\alpha} \right\} \quad (3.2)$$

here  $\delta \equiv \mu + \frac{J}{2}$  and the no-double-occupancy constraint is imposed by the potential  $u_{i,j}$ , defined as follows:

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<sup>7</sup>Eq. 3.2 can be derived from 3.1 by using the completeness relations for Pauli matrices to rewrite the spin term and by adding the time derivative term.

$$u_{i,j} = \begin{cases} +\infty, & \text{if } i=j \\ -\frac{J}{4}, & \text{if } i,j \text{ are n.n.} \\ 0 & \text{otherwise} \end{cases}$$

in this case the grand-canonical partition function can be written in terms of the action in eq. 3.2:

$$\Xi(\beta, \mu) = \int \mathcal{D}\Psi \mathcal{D}\Psi^* e^{-S(\Psi, \Psi^*)}$$

Moreover, we can use a Hubbard-Stratonovich transformation to decouple the quartic interaction in 3.2, obtaining:

$$S_{t/J} = \int_0^\beta d\tau \left\{ \sum_{\langle i,j \rangle} \left( \frac{2}{J} X_{\langle ij \rangle}^* X_{\langle ij \rangle} + [(-t + X_{\langle ij \rangle}^*) \Psi_{i,\alpha}^* \Psi_{j,\alpha} + h.c.] \right) + \sum_i \Psi_{i,\alpha}^* (\partial_0 + \delta) \Psi_{i,\alpha} + \sum_{i,j} u_{i,j} \Psi_{i,\alpha}^* \Psi_{j,\beta}^* \Psi_{j,\beta} \Psi_{i,\alpha} \right\}$$

Before developing an effective treatment for the  $t/J$  model it is worth noting that the theory is invariant under a global  $SU(2) \times U(1)$  group of symmetry. The  $SU(2)$  symmetry is due to the invariance for spatial rotations of the spin: a global rotation of spins will leave the  $\mathbf{S}_i \cdot \mathbf{S}_j$  scalar products invariant. On the other hand the  $U(1)$  symmetry is due to global charge conservation and corresponds to the action being left unchanged when multiplying each fermionic field for a constant phase factor.



## Chapter 4

# A gauge approach to cuprates

The aim of this chapter is to introduce the theoretical framework and approximations starting from which an effective action for the system will be derived. Through this effective treatment of the  $t/J$  model holon pairing, spinon pairing and ultimately superconductivity will be studied in subsequent chapters. For a more thorough discussion the reader is referred to the original papers, chiefly [29] and [7].

### 4.1 $SU(2) \times U(1)$ Chern-Simons bosonization

Bosonization is a procedure through which a system of interacting fermions can be transformed in a completely equivalent boson system. For one-dimensional systems the Jordan-Wigner bosonization achieves this result by using the following mapping:

$$c_j^\dagger \longrightarrow a_j^\dagger e^{-i\pi \sum_{l < j} a_l^\dagger a_l} \quad (4.1)$$

where  $c_j$  is a fermionic operator and  $a_j$  is a hard-core bosonic operator. The intuitive concept behind eq. 4.1 is that the new bosonic operator, to correctly re-implement the original statistics, has to be attached to a “string”, i.e. an object which counts, starting from  $-\infty$ , how many exchanges the

fermionic operator went through and restores the correct statistics.

The basic idea behind eq. 4.1 can be extended to higher dimensionality systems, at the expense of introducing one or more gauge fields which will provide the “counting factor” in eq. 4.1. Such a scheme is known as Chern-Simons bosonization. Provided that the following conditions hold:

- The original fermionic theory is described in terms of spin  $\frac{1}{2}$  non-relativistic hard core fermion fields in 2D position space.
- The fermions interact through a two-body spin-independent potential.
- An external abelian gauge field  $A$  is minimally coupled to the action.<sup>1</sup>

one is allowed to use a  $U(1) \times SU(2)$  Chern-Simons bosonization scheme, which will rewrite the theory as a function of newly introduced  $\Phi_\alpha(x)$  bosonic fields, while introducing at the same time a  $U(1)$  gauge field,  $B_\mu$  and a  $SU(2)$  gauge field,  $V_\mu \equiv V_\mu^a \frac{\sigma^a}{2}$ .

More specifically our bosonization scheme provides the following “recipe” to rewrite the theory in terms of bosons:

- The action for the system has to be coupled to the newly introduced gauge fields, and a kinetic term for the gauge fields must be added:

$$S(\Psi, \Psi^* | A) \longrightarrow S(\Phi, \Phi^*, A + B + V) + k_{U(1)} S_{C.S.}(B) + k_{SU(2)} S_{C.S.}(V) \quad (4.2)$$

for a suitable choice of the real coefficients  $k_{U(1)}$  and  $k_{SU(2)}$  and suitable boundary conditions<sup>2</sup>. The gauge kinetic terms appearing in the bosonic action are:

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<sup>1</sup>The following notation will be used:  $S(\Psi, \Psi^* | A)$  is the action obtained from  $S(\Psi, \Psi^*)$  by minimally coupling  $A$ .

<sup>2</sup>The choice of the coefficients which determines the statistics of the  $\Phi$  fields, will be discussed later. For a thorough discussion of the choice of the coefficients and of the boundary conditions see [30].



$$S_{\text{C.S.}}(B) = \frac{1}{4\pi i} \int_0^\beta dx^0 \int d^n x \epsilon^{\mu\nu\rho} B_\mu \partial_\nu B_\rho$$

$$S_{\text{C.S.}}(V) = \frac{1}{4\pi i} \int_0^\beta dx^0 \int d^n x \epsilon^{\mu\nu\rho} \text{tr} \left[ V_\mu \partial_\nu V_\rho + \frac{2}{3} V_\mu V_\nu V_\rho \right]$$

- The fermionic fields in the action in eq. 4.2 are to be replaced by non-local bosonic fields bound to a string:

$$\Psi_\alpha(x) \longrightarrow \Phi_\alpha(\gamma_x|B, V) \equiv e^{i \int_{\gamma_x} B} P \left( e^{i \int_{\gamma_x} V} \right)_{\alpha\beta} \Phi_\beta(x)$$

$$\Psi_\alpha^*(x) \longrightarrow \Phi_\alpha^*(\gamma_x|B, V) \equiv \Phi_\beta^*(x) e^{i \int_{\gamma_x} B} P \left( e^{i \int_{\gamma_x} V} \right)_{\beta\alpha}$$

where  $\gamma_x$  is a string connecting point  $x$  to a fixed point placed at infinity and  $P(\#)$  denotes path-ordering.

- Finally, the partition function for the system is to be rewritten using the following **bosonization formula**:

$$\int \mathcal{D}\Psi \mathcal{D}\Psi^* e^{-S(\Psi, \Psi^*|A)} = \frac{\int \mathcal{D}B \mathcal{D}V \int \mathcal{D}\Phi \mathcal{D}\Phi^* e^{-[S(\Phi, \Phi^*|A+B+V) + 2S_{\text{C.S.}}(B) + S_{\text{C.S.}}(V)]}}{\int \mathcal{D}B \mathcal{D}V e^{-[2S_{\text{C.S.}}(B) + S_{\text{C.S.}}(V)]}}$$

where an adequate gauge fixing is implied in the right-hand side and the coupling constants in eq. 4.2 have been chosen to be:

$$k_{U(1)} = +2 \quad k_{SU(2)} = +1 \quad (4.3)$$

To sum up, using the Chern-Simons bosonization scheme one can, upon specific conditions, rewrite a fermionic in terms of non-local bosonic fields, by introducing a number of additional minimally coupled gauge fields.

We still have to justify the choice of the gauge group and of the coupling constants, which, at this point, may seem quite arbitrary.

To justify the choice of the gauge group  $G = SU(2) \times U(1)$  it is worth showing the  $SU(2)$  and  $U(1)$  naturally gauge, respectively, the spin and charge degrees of freedom. To see that, observing that the  $B_0$  and  $V_0$  terms appear only linearly in the action, one can integrate them out obtaining the following constraints:

$$j_0(x) = \frac{1}{2\pi} \epsilon_{0\nu\rho} W^{\nu\rho}(x) \quad (4.4)$$

where  $j_0$  is density of the matter field, and  $W$  is the abelian (non-abelian) field strength for  $B$  ( $V$ ). Taking for instance  $B_\mu$  eq. 4.4 could also be rewritten as  $\nabla \times \mathbf{B}(x) \sim \rho(x)$ , meaning that a magnetic-like charge is assigned to every matter particle, and that  $B$  can be indeed regarded as a magnetic field.

On the other side, the choice in eq. 4.3 can be justified by noting that this choice of coefficients when applying a 2D  $\rightarrow$  1D dimensional reduction provides MFA results which are in accordance with the exact 1D solution for the  $t/J$  model, obtained by Bethe-Ansatz or Conformal Field Theory (see [31] and citations therein).

## 4.2 Spin-charge separation

As noted in the introduction it has been argued that the fundamental excitations in cuprates should be particles carrying only charge or only spin, called, respectively, holons and spinons; this assertion has been verified for one-dimensional systems ([5] and [6]) and hints in this direction have also been found for higher-dimensional systems ([32]). Starting from these remarks, the bosonic field  $\Phi_{x\alpha}$  can be formally be decomposed, through polar decomposition, as the product of two fields

$$\Phi_{x\alpha} = E_x \Sigma_{x\alpha} \quad (4.5)$$

where  $E_x$  is a complex scalar boson describing the charge degrees of freedom, while  $\Sigma_\alpha$  is 2-component spin  $\frac{1}{2}$  complex boson describing the spin degrees of freedom. The following constraint is imposed on  $\Sigma_\alpha$ :

$$\Sigma_{x\alpha}^* \Sigma_{x\alpha} = 1 \quad (4.6)$$

The field  $E_x$  carries 2 degrees of freedom,  $\Sigma_\alpha$  carries 4 degrees of freedom; the constraint in eq. 4.6 takes one degree of freedom away and we are left with 5 degrees of freedom. The original theory, when expressed in terms of fermionic fields, had only 4 degrees of freedom, so some new invariance must have been added to the theory while separating spin and charge. It is indeed easily seen that the polar decomposition introduces a local  $U(1)$  gauge invariance leaving  $\Phi_{x\alpha}$  and all other observables invariant:

$$\begin{cases} E_j \longrightarrow E_j e^{i\Lambda_j} \\ \Sigma_{j\alpha} \longrightarrow \Sigma_{j\alpha} e^{-i\Lambda_j} \end{cases} \quad \Lambda_j \in [0, 2\pi[$$

When fixing this gauge symmetry (which we will call  $h/s$  symmetry and will leave, for the moment, exact) one restores the correct counting of the degrees of freedom.

As already pointed out, the  $B_\mu$  gauge field is naturally associated to the charge degree of freedom, and  $V_\mu$  is naturally associated the spin degree of freedom, so that it is convenient to formally bind the charged  $E$  field to the  $B_\mu$  string and the  $\Sigma$  field to the  $V_\mu$  string in the following way:

$$\Phi_\alpha(\gamma_x | B, V) = \left[ e^{i \int_{\gamma_x} B} E_x \right] \left[ P \left( e^{i \int_{\gamma_x} V} \right)_{\alpha\beta} \Sigma_{x\beta} \right]$$

Moreover one can further justify this decomposition by noting that, when taken singularly,  $e^{i \int_{\gamma_x} B} E_x$  and  $P \left( e^{i \int_{\gamma_x} V} \right)_{\alpha\beta} \Sigma_{x\beta}$  are gauge invariant objects by itself with semionic statistics<sup>3</sup>.

<sup>3</sup>A semion is an object which acquires a  $\pm i$  factor upon exchange of two identical particles. When regarding the statistical factor as a phase on the unitary circle, the

At last, it is convenient to transform the charge-like excitations  $E_j$  in hole-like excitations; this can be achieved by performing the following substitutions

$$\begin{cases} E_j \longrightarrow H_j^* \\ E_j^* \longrightarrow H_j \end{cases} \quad (4.7)$$

where  $H$  and  $H^*$  are Grassman fields. The statistical flux bound to  $E_j$  has to be changed, too, namely setting  $k_{U(1)} = -2$ . Finally, the theory is described in terms of hole-like excitations, called **holons**, and charge-less spin  $\frac{1}{2}$  particles, which we will call **spinons**.

As a side effect, the repulsive hard-core potential or the Gutzwiller projector are no longer needed, as  $H_j$  is a spinless fermionic field which automatically enforces the no-double occupancy constraint.

As final result of this section one can rewrite the action for the system in terms of holons and spinons as follows:

$$\Xi(\beta, \mu) = \int \mathcal{D}H \mathcal{D}H^* \mathcal{D}\Sigma_\alpha \mathcal{D}\Sigma_\alpha^* \mathcal{D}B \mathcal{D}V \mathcal{D}X e^{-S(H, H^*, \Sigma_\alpha, \Sigma_\alpha^*, B, V, X)} \delta(\Sigma^* \Sigma - 1) \quad (4.8)$$

and integrate out the  $X$  auxiliary variable, so that the Euclidean action  $S(H, H^*, \Sigma, \Sigma^*, B, V)$  now reads:

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semion statistics are halfway between fermion and boson statistics, hence the name.

$$\begin{aligned}
S = \int_0^\beta d\tau \left\{ \left[ H_j^* \left( \partial_0 - iB_0(j) - \left( \mu + \frac{J}{2} \right) \right) H_j + iB_0(j) + \right. \right. \\
+ (1 - H_j^* H_j) \Sigma_{j\alpha}^* (\partial_0 + iV_0(j))_{\alpha\beta} \Sigma_{j\beta} \left. \right] + \\
\sum_{\langle ij \rangle} \left[ \left( -t H_j^* e^{i \int_{\langle ij \rangle} B} H_i \Sigma_{i\alpha}^* \left( P e^{i \int_{\langle ij \rangle} V} \right)_{\alpha\beta} \Sigma_{j\beta} + h.c. \right) + \right. \\
+ \left. \frac{J}{2} (1 - H_i^* H_i) (1 - H_j^* H_j) \left( \left| \Sigma_{i\alpha}^* \left( P e^{i \int_{\langle ij \rangle} V} \right)_{\alpha\beta} \Sigma_{j\beta} \right|^2 - \frac{1}{2} \right) \right] \left. \right\} \\
- 2S_{C.S.}(B) + S_{C.S.}(V)
\end{aligned} \tag{4.9}$$

### 4.3 Gauge fixings

It is clear that in order to give physical meaning to the functional integration in eq. 4.8 one has to first gauge-fix the additional gauge symmetries of the theory, namely:

- The  $U(1)$   $h/s$  symmetry, introduced by the spin-charge separation.
- The  $SU(2)$  symmetry, corresponding to the spin degrees of freedom.
- The  $U(1)$  symmetry, corresponding to the charge degree of freedom.

Explicitely these symmetries correspond to the following transformations:

$$U(1)_{h/s} : \begin{cases} H_j \longrightarrow H_j e^{i\Lambda_j} \\ \Sigma_{j\alpha} \longrightarrow \Sigma_{j\alpha} e^{i\Lambda_j} \end{cases} \quad \Lambda_j \in [0, 2\pi[ \tag{4.10}$$

$$SU(2)_V : \begin{cases} \Sigma_j \longrightarrow R^\dagger(j) \Sigma_j \\ V_\mu(x) \longrightarrow R^\dagger(x) V_\mu(x) R(x) + R^\dagger \partial_\mu(x) R(x) \end{cases} \quad R(x) \in SU(2) \tag{4.11}$$

$$U(1)_B : \begin{cases} H_j \longrightarrow H_j e^{i\zeta_j} \\ B_\mu(x) \longrightarrow B_\mu(x) + \partial_\mu \zeta(x) \end{cases} \quad \zeta_j \in [0, 2\pi[ \quad (4.12)$$

The  $h/s$  symmetry is left explicit and will be fixed at a later time. The other two symmetries are fixed by the following gauge choices; for  $B_\mu$  the Coulomb gauge is chosen:

$$\partial_\mu B^\mu = 0 \quad \mu = 1, 2$$

while the  $SU(2)$  is fixed by imposing a fixed configuration for the spinons, the ‘‘Néel gauge condition’’, leaving the  $V$  gauge field unconstrained:

$$\Sigma_j = \sigma_x^{|j|} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \Sigma_j^* = (1, 0) \sigma_x^{|j|} \quad (4.13)$$

This ‘‘gauge choice’’ is particularly convenient as the low-energy physics of spinons are dominated by an anti-ferromagnetic background which eq. 4.13 automatically enforces; obviously having fixed the spinon configuration the relevant degrees of freedom are transferred to the gauge field  $V$  and integrating over this field provides the necessary fluctuations around the Néel anti-ferromagnetic configuration. The integration over  $V$  is then split in the integration over a field  $V^{(c)}$  constrained by a Coulomb gauge condition ( $\partial_\mu V^{(c)} = 0, \mu = 1, 2$ ) and over its  $SU(2)$  gauge transformations, expressed with an  $SU(2)$ -valued scalar field  $g$ :

$$V_a = g^\dagger V_a^{(c)} g + g^\dagger \partial_a g \quad a = 0, 1, 2$$

Fixing the gauge also provides some additional constraints for the gauge fields. Specifically, by observing (as done in deriving eq. 4.4) that the time components of the gauge fields appear linearly in the action, one can carry out the functional integration, obtaining a  $\delta(\#)$  function which imposes a

constraint on the other components of the field. For  $B_\mu$  this procedure leads to:

$$B_\mu = \bar{B}_\mu + \delta B_\mu \quad \delta B_\mu(x) = \frac{1}{2} \sum_j H_j^* H_j \partial_\mu \arg(x - j) \quad (4.14)$$

$\bar{B}_\mu$  being a static component giving a  $\pi$ -flux phase for plaquette, i.e.  $e^{i \int_{\partial p} \bar{B}} = 1$ . It is worth noting that a configuration for the  $\bar{B}_\mu$  field which respects the  $\pi$ -flux constraint must have a periodicity of  $2 \times 2$  lattice site and be arranged in a staggered way; a configuration which respects the aforementioned flux constraint is not unique, its complete definition being equivalent to completing the gauge fixing procedure for  $B_\mu$ ; our choice is depicted in fig. 4.1. The additional periodicity for the  $\bar{B}_\mu$  field effectively defines the size of the magnetic Brillouin zone and will come into play when analyzing holon pairing in chapter 5.

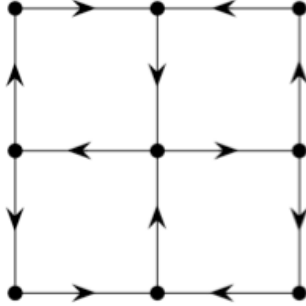


Figure 4.1: The staggered configuration for the  $\pi$ -flux  $\bar{B}$  field; each link represents a  $\pm \frac{\pi}{4}$  phase, the sign being defined by the arrow direction. A  $\pm\pi$  flux passes through each plaquette.

As far as the  $SU(2)$   $V_\mu$  field is concerned, the integration yields:

$$V_\mu^{(c)} = \sum_j (1 - H_j^* H_j) \left( \sigma_x^{|j|} g_j^\dagger \frac{\sigma_a}{2} g_j \sigma_x^{|j|} \right)_{11} \partial_\mu \arg(x - j) \sigma_a \quad (4.15)$$

## 4.4 Optimization of spinon configuration

The aim of this section is finding a holon-dependent spinon configuration  $g^m(H, H^*)$  which maximizes the partition function. This procedure can be justified by noting that the spinon fluctuations have a much shorter time scale than the holes, so that finding  $g^m$  as a function of the holon configuration kind of resembles separating the fast and slow variables of the system.

Provided that the following identifications are made:

$$iA_j \sim \left( \sigma_x^{[j]} g_j^\dagger \partial_0 g_j \sigma_x^{[j]} \right)_{11}$$

$$U_{\langle ij \rangle} \sim e^{-i \int_{\langle ij \rangle} (\bar{B} + \delta B)} \left[ \sigma_x^{[i]} g_i^\dagger \left( P e^{i \int_{\langle ij \rangle} V^{(c)}} \right) g_j \sigma_x^{[j]} \right]_{11}$$

after fixing the gauge and imposing the constraints in eq. 4.14 and eq. 4.15 the action for the system can be recast as  $S = S_1 + S_2$ , where:

$$S_1 = (H, H^*, A, U) = \int_0^\beta d\tau \left\{ \sum_j [H_j^* (\partial_0 + \delta) H_j + i (1 - H_j^* H_j) A_j] \right. \\ \left. + \sum_{\langle ij \rangle} (-t H_i^* U_{\langle ij \rangle} H_j + h.c.) \right\}$$

$$S_2 = (H, H^*, U) = \int_0^\beta d\tau \sum_{\langle ij \rangle} (1 - H_i^* H_i) (1 - H_j^* H_j) \left( |U_{\langle ij \rangle}|^2 - \frac{1}{2} \right)$$

A theorem due to Marchetti, Su and Yu [29] establishes an upper bound for the partition function of the system described by  $S = S_1 + S_2$ , more specifically let:

$$\Xi(A, U) = \int \mathcal{D}H \mathcal{D}H^* e^{-S(H, H^*, A, U)}$$

it can be proven that:

$$|\Xi(A, U)| \leq \int \mathcal{D}H \mathcal{D}H^* e^{-[S_1(H, H^*, 0, \hat{U}) + S_2(H, H^*, 0)]}$$



where  $\hat{U}$  is the time independent configuration maximizing

$$\int \mathcal{D}H\mathcal{D}H^* e^{-[S_1(H,H^*,0,U)+S_2(H,H^*,0)]} \Big|_{\partial_0 U=0}$$

It can be shown (a complete demonstration of the theorem stated above can be found in [29], here the main results will be briefly summarized) that it is possible to find a spinon configuration  $g^m$  which saturates this bound on average, and then one can recover an exact treatment by adding the fluctuations around  $g^m$ .

Following the notation used in the original article, a generic spinon configuration is then:

$$g_j = \bar{g}_j R_j \tilde{g}_j = e^{-\frac{i}{2} \sum_{i \neq j} (-1)^i \sigma_z \arg(i-j)} R_j e^{i \frac{\pi}{2} (-1)^{|j|} \sigma_y H_j^* H_j}$$

where the matrix  $R_j \in SU(2)$  represents the fluctuations, so that the optimal configuration is given by  $R_j \equiv \mathbb{1}$ . Moreover it is convenient to represent the fluctuations in  $CP^1$  form, i.e. parametrizing the  $R_j \in SU(2)$  as:

$$R_j = \begin{pmatrix} b_{j1} & -b_{j2}^* \\ b_{j2} & b_{j1}^* \end{pmatrix} \quad b_{j\alpha}^* b_{j\alpha} = 1$$

where  $b_\alpha$  is a spin  $\frac{1}{2}$  field obeying the constraint  $b_\alpha^* b_\alpha = 1$  at every site. In addition to that, as a side effect of the spinon configuration optimization procedure it can be seen that, as  $g^m$  can be chosen to be diagonal at sites without any holons, the  $SU(2)$  field in eq. 4.15 can be simplified as follows:

$$V^{(c)}(x) = \sum_j (1 - H_j^* H_j) \frac{(-1)^{|j|}}{2} \partial_\mu \arg(x-j) \sigma_z$$

and can then be recast as  $V^{(c)} = \bar{V} + \delta V$ , where  $\delta V$  is a fast-oscillating term and  $\bar{V}$  is defined by:

$$\bar{V} = - \sum_j H_j^* H_j \frac{(-1)^{|j|}}{2} \partial_\mu \arg(x-j) \sigma_z \quad (4.16)$$

From a physical point of view eq. 4.16 describes a gas of vortices centered on each holon site, with a +1 (-1) topological charge if the site is even (odd); to justify this assertion one can imagine taking the curl of  $\bar{V}$  when only one holon is present in the system at site  $j$ , observing that in this case:

$$\epsilon^{\mu\nu} \partial_\mu \bar{V}_\nu(i-j) \sim \delta(i-j)$$

At the end of the optimization procedure we can finally write an Euclidean action for the system as  $S = S_h + S_s$  where:

$$S_h = \int_0^\beta d\tau \left\{ \sum_j H_j^* \left[ \partial_0 - \left( \sigma_x^{|j|} R_j^\dagger \partial_0 R_j \sigma_x^{|j|} \right)_{11} - \delta \right] H_j + \right. \\ \left. + \sum_{\langle ij \rangle} \left[ -t H_j^* e^{i \int_{\langle ij \rangle} \delta B} H_i \left( \sigma_x^{|i|} R_i^\dagger P e^{i \int_{\langle ij \rangle} (\bar{V} + \delta V)} R_j \sigma_x^{|i|} \right)_{11} + h.c. \right] \right\} \quad (4.17)$$

$$S_s = \int_0^\beta d\tau \left\{ \sum_j \left( \sigma_x^{|j|} R_j^\dagger \partial_0 R_j \sigma_x^{|j|} \right)_{11} + \right. \\ \left. + \sum_{\langle ij \rangle} \frac{J}{2} (1 - H_i^* H_i) (1 - H_j^* H_j) \left[ \left| \left( \sigma_x^{|i|} R_i^\dagger P e^{i \int_{\langle ij \rangle} (\bar{V} + \delta V)} R_j \sigma_x^{|i|} \right)_{11} \right|^2 - \frac{1}{2} \right] \right\} \quad (4.18)$$

where  $\delta V \equiv V^{(c)} - \bar{V}$  and it is understood that when constructing the partition function from eq. 4.17 and 4.18 one integrates over  $H$ ,  $H^*$ ,  $R$  and  $R^\dagger$ , the latter two taking values in  $SU(2)$ .

## 4.5 Approximations and effective action for spinons

Up to this point the treatment has always be kept exact<sup>4</sup>: the theory has been conveniently rewritten in terms of different variables which will allow us to put in practice a sensible mean-field approximation. The main approximation consists in neglecting the feedback of spinon fluctuations in the gauge field  $V$ , i.e. setting:

$$\delta V = 0 \tag{4.19}$$

It has been argued [33] that by neglecting the fluctuations in the gauge fields one does not affect in an essential way the physics of the electrons; however the statistics of the spinons are affected by the constraint in eq. 4.19, namely the gauge-invariant spinon field

$$P \left( e^{i \int_{\gamma_j} V} \right) \Sigma_j = e^{i \int_{\gamma_j} (\bar{V} + \delta V)} \bar{g}_j R_j \sigma_x^{|j|} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

is no longer a semion. For consistency, as the product of a spinon and a holon has to be a fermion, one also has to neglect the holon feedback to the gauge field  $B_\mu$ , i.e.:

$$\delta B = 0 \tag{4.20}$$

also changing the statistics for the gauge-invariant holon field  $e^{-i \int_{\gamma_j} B} H_j$ , and restoring back the fermionic statistics for the electron.

In order to derive the low-energy physics of this model one can conveniently define the following matrix, with each entry defined on a lattice link:

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<sup>4</sup>Except for the assumptions of small  $\delta$ , large  $\beta$  in the derivation of the optimal spinon configuration  $g^m$ .

$$\begin{aligned}
R_i^\dagger e^{i \int_{\langle ij \rangle} \bar{V}} R_j &= \begin{pmatrix} \alpha_{\langle ij \rangle} b_{i1}^* b_{j1} + \alpha_{\langle ij \rangle}^* b_{i2}^* b_{j2} & -\alpha_{\langle ij \rangle} b_{i1}^* b_{j2} + \alpha_{\langle ij \rangle}^* b_{i2}^* b_{j1} \\ -\alpha_{\langle ij \rangle} b_{i2} b_{j1} + \alpha_{\langle ij \rangle}^* b_{i1} b_{j2} & \alpha_{\langle ij \rangle} b_{i2} b_{j2} + \alpha_{\langle ij \rangle}^* b_{i1} b_{j1} \end{pmatrix} \equiv \\
&\equiv \begin{pmatrix} AM_{ij} & -RVB_{ij} \\ RVB_{ij}^* & AM_{ij}^* \end{pmatrix}
\end{aligned} \tag{4.21}$$

where  $\alpha_{\langle ij \rangle} \equiv e^{\frac{i}{2} \int_{\langle ij \rangle} \bar{V}_z}$ . Moreover one can rewrite the spinon and holon actions in eq. 4.17 and 4.18, writing the holon hopping term as:

$$t \sum_{\langle ij \rangle} H_j^* e^{i \int_{\langle ij \rangle} \bar{B}} H_i AM_{ij} \tag{4.22}$$

and the spinon Heisenberg term as:

$$\frac{J}{2} \sum_{\langle ij \rangle} (1 - H_i^* H_i) (1 - H_j^* H_j) \left( |RVB_{ij}|^2 - \frac{1}{2} \right) \tag{4.23}$$

This duality, i.e. the presence of both  $RVB$ -like and  $AM$ -like factors will be discussed in detail in section 4.6 and is peculiar of our  $U(1) \times SU(2)$  model; for now we only note that, by definition, the identity  $|AM_{ij}|^2 + |RVB_{ij}|^2 = 1$  holds.

It is clearly seen that the matrix in eq. 4.21 contains the fundamental features of holon and spinon dynamics. As a last step before being able to write down an effective action for the spinons and holons, as customary in antiferromagnetic systems, one wants to separate the antiferromagnetic and ferromagnetic fluctuations by introducing, respectively, the fields  $\vec{Q}$  and  $\vec{L}$ , defined on a Néel sublattice<sup>5</sup> as follows:

$$b_{j\alpha}^* \vec{\sigma}_{\alpha\beta} b_{j\beta} \sim \vec{\Omega}_j + (-1)^{|j|} \epsilon \vec{L}_j \tag{4.24}$$

---

<sup>5</sup>We need to define  $\vec{Q}$  and  $\vec{L}$  on a sublattice to maintain the right number of degrees of freedom.

and by the conditions:  $\vec{\Omega}_j^2 = f \sim 1$  and  $\vec{\Omega} \cdot \vec{L} = 0$ . At the same time the system is rescaled to a lattice spacing  $\epsilon \ll 1$ . This allows us to rewrite the  $\alpha_{ij}$  link variable by Taylor-series expansion using the lattice spacing  $\epsilon$  as parameter; up to the second order the expansion reads:

$$e^{-i \int_{\langle ij \rangle} \bar{V}_z} = 1 + \epsilon (-i \bar{V}_z)(j) + \frac{\epsilon^2}{2} (-i \bar{V}_z)^2(j) + O(\epsilon^3)$$

The Heisenberg term for spinons (from eq. 4.18) in the new variables on the rescaled lattice now reads:

$$\frac{J}{2} \sum_{\langle ij \rangle} (1 - H_i^* H_i) (1 - H_j^* H_j) \left( |AM_{ij}|^2 - \frac{1}{2} \right) = \frac{J}{2} \sum_{\langle ij \rangle} \left\{ \frac{1}{2} \left( \frac{\vec{\Omega}_i - \vec{\Omega}_j}{\epsilon} \right)^2 + 2\vec{L}_j^2 + \bar{V}_z^2(j) \left[ (\Omega_{jx})^2 + (\Omega_{jy})^2 \right] \right\}$$

where the holon contribution in the l.h.s. has been treated as constant in MFA and has been included, to the lowest relevant order in  $\delta$ , by redefining  $J \rightarrow \tilde{J} \equiv J(1 - 2\delta)$ . On the other hand, the time-derivative term of eq. 4.18 reads:

$$- \left( \sigma_x^{|j|} R_j^\dagger \partial_0 R_j \sigma_x^{|j|} \right)_{11} = \frac{\epsilon}{2} \vec{L}_j \cdot \left( \vec{\Omega}_j \times \partial_0 \vec{\Omega}_j \right) + O(\epsilon^2)$$

Integrating out the  $\vec{L}$  variables, taking the  $\epsilon \rightarrow 0$  continuum limit and replacing  $\bar{V}$  with its statistical average, one can derive an effective action for spinons<sup>6</sup>:

$$S = \int_0^\beta d\tau \int d^2x \left[ \left( \partial_0 \vec{\Omega} \right)^2 + v_s^2 \left( \partial_\mu \vec{\Omega} \right)^2 + \frac{2}{3} \left( \vec{\Omega} \right)^2 \langle \bar{V}_z^2 \rangle \right] \quad \mu = 1, 2$$

with  $g \equiv \frac{8}{\tilde{J}}$  and  $v_s \equiv \sqrt{2} \tilde{J} a$ . Finally, a spin  $\frac{1}{2}$  bosonic hard-core field,  $z_\alpha$  is introduced to rewrite  $\vec{\Omega}$  in  $CP^1$  form:

$$\vec{\Omega} = z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta \quad z_\alpha^* z_\alpha = f \quad (4.25)$$

<sup>6</sup>An unphysical topological  $\theta$ -term has been left out and we assume rotational invariance for the system.

In terms of these newly-introduced fields an effective action for spinons can be written as the action of a non-linear  $\sigma$ -model:

$$\mathcal{S}_s = \frac{1}{g} \int_0^\beta d\tau \int d^2x \left[ |(\partial_0 - iA_0) z_\alpha|^2 - v_s^2 |(\partial_\mu - iA_\mu) z_\alpha|^2 + m_s^2(\delta) z_\alpha^* z_\alpha \right] \quad (4.26)$$

An important feature appearing in the effective action is the emergent self-generated  $U(1)$  field which, as we will see, is related to the continuum version of the  $h/s$  symmetry:

$$A_\mu \sim z_\beta^* \partial_\mu z_\beta \quad (4.27)$$

While deriving the effective action for holons it will be clear that this field effectively “binds” holons and spinons, as it is also evident by looking at the transformations in eq. 4.10, upon which the spinon and holon fields transform with opposite charge. On the other side the mass in eq. 4.26 is generated by the lowest term which couples the  $SU(2)$  gauge field and the spin, i.e.  $(\vec{\Omega})^2 (\bar{V}_z)^2$  when  $(\bar{V}_z)^2$ , dependent on the holon configuration, is replaced by its statistical average:

$$\langle \bar{V}_z^2 \rangle = m_s^2 \sim -\delta \ln \delta$$

which defines the mass term.

## 4.6 Mean-field hamiltonian for the t/J model

For certain applications it will be more convenient working in the Hamiltonian formalism, aim of this section is writing down a MFA hamiltonian for the system. Introducing the  $z_\alpha, z_\alpha^*$  fields as done in the previous section, and adopting the notation in [7] one can define the entries of the matrix in eq. 4.21 as:

$$R_i^\dagger e^{i \int_{\langle ij \rangle} \bar{V}} R_j = \begin{pmatrix} \chi_{ij}^s & -\Delta_{ij}^s \\ \Delta_{ij}^{s*} & \chi_{ij}^{s*} \end{pmatrix}$$

and formally rewrite the actions in eq. 4.17 and 4.18 as:

$$S_h(H, H^*, b, b^\dagger) = \int_0^\beta d\tau \left\{ \sum_j H_j^* \left( \partial_0 - (b_{j\alpha}^* \partial_0 b_{j\alpha})^{\#(j)} - \delta \right) H_j + \right. \\ \left. + t \sum_{\langle ij \rangle} \left( H_j^* e^{i \int_{\langle ij \rangle} \bar{V}} H_i \chi_{ij}^s + h.c. \right) \right\} \quad (4.28)$$

$$S_s(H, H^*, b, b^\dagger) = \int_0^\beta d\tau \left\{ \sum_j (b_{j\alpha}^* \partial_0 b_{j\alpha})^{\#(j)} \frac{J}{2} \sum_{\langle ij \rangle} (1 - H_i^* H_i) (1 - H_j^* H_j) \left( |\Delta_{ij}^s|^2 - \frac{1}{2} \right) \right\} \quad (4.29)$$

having defined:

- The Affleck-Marston (AM) term:  $\chi_{ij}^s \equiv \left( z_i^* e^{iV_{ij}^N} z_j \right)^{\#(i)}$
- The Resonating Valence Bond (RVB) term:  $\Delta_{ij}^s \equiv \epsilon^{\alpha\beta} z_{i\alpha} \left( e^{iV_{ij}^N \sigma_z} z_j \right)_\beta$

where the following shorthands have been used:  $V_{ij}^N = \int_i^j dx^\mu \bar{V}_\mu^z(\mathbf{x}) \approx \bar{V}_\mu^z \left( \frac{\mathbf{i}+\mathbf{j}}{2} \right) a^\mu$ ,  $a$  denotes the lattice constant and  $\#(i)$  is the complex conjugation if  $i$  belongs to the odd Néel sublattice. As previously briefly stated these two terms are a peculiar feature of our  $U(1) \times SU(2)$  model; in fact both an RVB and an AM factor appear at the same time, as opposed to the slave boson/fermion approaches, the *AM* term regulating the  $t$  hopping term of the  $t/J$  model and the *RVB* term regulating the  $J$  Heisenberg term. The gauge field  $V_\mu$ , being in the definitions of both  $\chi_{ij}^s$  and  $\Delta_{ij}^s$ , regulates both of the two relevant quantities of the  $t/J$  model.

The Hamiltonian for the system just discussed is now easily written by discarding the temporal derivatives and introducing the field operators, as:

$$\begin{aligned}
\hat{H}_{t/J} \approx & t \sum_{\langle i,j \rangle} \hat{h}_j^\dagger e^{i\bar{B}_{ij}} \hat{h}_i \hat{\chi}_{ij}^s + h.c. + \\
& + \mu \sum_i \hat{h}_i^\dagger \hat{h}_i + \frac{J}{2} \sum_{\langle i,j \rangle} \left( 1 - \hat{h}_i^\dagger \hat{h}_i - \hat{h}_j^\dagger \hat{h}_j \right) \hat{\Delta}_{ij}^s \hat{\Delta}_{ij}^{s\dagger} + \hat{h}_i^\dagger \hat{h}_i \hat{h}_j^\dagger \hat{h}_j \hat{\Delta}_{ij}^s \hat{\Delta}_{ij}^{s\dagger}
\end{aligned} \tag{4.30}$$

with the obvious meaning of the  $\hat{\Delta}_{ij}^s$  and  $\hat{\chi}_{ij}^s$  operators, straightforwardly derived from their field version.

## 4.7 Effective action for holons

An effective action for the holon part can be obtained can be obtain exactly in the same way as for spinons; namely by separating the antiferromagnetic and ferromagnetic contributions while rescaling the lattice, integrating out the ferromagnetics degrees of freedom and taking the continuum limit.

Thanks to the slowly-varying nature of the  $\bar{V}_\mu$  field, one can treat the  $AM_{ij}$  factor, as defined by eq. 4.21, in MFA by approximating as follows:

$$\langle \alpha_{\langle ij \rangle} b_{i1}^* b_{j1} + \alpha_{\langle ij \rangle}^* b_{i2}^* b_{j2} \rangle \approx b_{i1}^* b_{i1} + b_{i2}^* b_{i2} = 1 \tag{4.31}$$

In the aforementioned approximation the holon action in eq. 4.17 reads:

$$\begin{aligned}
S_h = & \int_0^\beta d\tau \left( \sum_j H_j^* \left( \partial_0 - (b_{j\alpha}^* \partial_0 b_{j\alpha})^{\#(j)} - \delta \right) H_j + \right. \\
& - t \sum_{\langle ij \rangle} e^{i \int_{\langle ij \rangle} \bar{B}} \left\{ \frac{H_i^* H_j - H_j^* H_i}{\epsilon} + \right. \\
& \left. \left. + (H_i^* H_j + H_j^* H_i) \left[ b_{i\alpha}^* \left( \frac{b_{j\alpha} - b_{i\alpha}}{\epsilon} \right) - \left( \frac{b_{j\alpha}^* - b_{i\alpha}^*}{\epsilon} \right) b_{j\alpha} \right]^{\#(j)} \right\} \right) + O(\epsilon)
\end{aligned} \tag{4.32}$$

The  $\bar{B}$  field, as the reader will remember, has been gauge-fixed to a staggered  $\pi$ -flux configuration, as in fig. 4.1. It is then convenient to redefine the field operators so that they are acting on four different sublattices, making



explicit the periodicity in the  $B_\mu$  field. Specifically, a lattice site  $(j_1, j_2)$  will belong to the sublattice:

- (1), if both  $j_1$  and  $j_2$  are even.
- (2), if both  $j_1$  is odd and  $j_2$  is even.
- (3), if both  $j_1$  is even and  $j_2$  is odd.
- (4), if both  $j_1$  and  $j_2$  are odd.

The theory can then be redefined in term of the restriction  $H_i$  of the holon field to the  $i$ -the sublattice; in terms of these fields the theory is described by the following  $4 \times 4$  matrix:

$$\begin{pmatrix} \partial_0 - z_\alpha^* \partial_0 z_\alpha - \delta & it(\partial_1 + z_\alpha^* \partial_1 z_\alpha) & -it(\partial_2 + z_\alpha^* \partial_2 z_\alpha) & 0 \\ it(\partial_1 - z_\alpha^* \partial_1 z_\alpha) & \partial_0 + z_\alpha^* \partial_0 z_\alpha - \delta & 0 & it(\partial_2 - z_\alpha^* \partial_2 z_\alpha) \\ -it(\partial_2 - z_\alpha^* \partial_2 z_\alpha) & 0 & \partial_0 + z_\alpha^* \partial_0 z_\alpha - \delta & it(\partial_1 - z_\alpha^* \partial_1 z_\alpha) \\ 0 & it(\partial_2 + z_\alpha^* \partial_2 z_\alpha) & it(\partial_1 + z_\alpha^* \partial_1 z_\alpha) & \partial_0 - z_\alpha^* \partial_0 z_\alpha - \delta \end{pmatrix}$$

in which the ferromagnetic contributions have been integrated out and the antiferromagnetic ones have been rewritten in terms of the newly-introduced fields  $z_\alpha$  as done in equations 4.24 and 4.25. With the usual choice for the  $\gamma$  matrices in two spatial dimensions  $\gamma_\mu = (\sigma_z, \sigma_y, \sigma_x)$ ,  $\mu = 0, 1, 2$ , and by further redefining the fields:

$$\Psi_1 = \begin{pmatrix} \Psi_1^{(A)} \\ \Psi_1^{(B)} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\pi}{4}} H^{(1)} + e^{i\frac{\pi}{4}} H^{(4)} \\ e^{-i\frac{\pi}{4}} H^{(3)} + e^{i\frac{\pi}{4}} H^{(2)} \end{pmatrix} \quad \Psi_2 = \begin{pmatrix} \Psi_2^{(A)} \\ \Psi_2^{(B)} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\pi}{4}} H^{(2)} + e^{i\frac{\pi}{4}} H^{(3)} \\ e^{-i\frac{\pi}{4}} H^{(4)} + e^{i\frac{\pi}{4}} H^{(1)} \end{pmatrix} \quad (4.33)$$

and  $\bar{\Psi}_r = \Psi_r^\dagger \gamma_0$ , one can create a theory, described by two spinors whose components are defined, respectively, on the even Néel sublattice and on the odd Néel sublattice. Labelling the even and odd sublattices respectively with  $A$  and  $B$  it is clear that:  $A = (1) + (4)$  and  $B = (2) + (3)$ , giving physical

meaning to the definitions in eq. 4.33. Such a theory makes manifest that the effective action for spinons is ultimately a theory of Dirac-like fermions, with charge  $\pm 1$  given by the Néel sublattice they are on. By taking the continuum limit ( $\epsilon \rightarrow 0$ ) the effective action for the holons is:

$$S_h = \int_0^\beta d\tau \int d^2x \sum_{r=1}^2 \bar{\Psi}_r [\gamma_0 (\partial_0 - \delta - e_r A_0) + v_F \gamma_\mu (\partial_\mu - e_r A_\mu)] \Psi_r \quad (4.34)$$

with the charge defined by:  $e_A = +1$ ,  $e_B = -1$  and  $\mu = 1, 2$ . Once again when writing the effective action the  $h/s$  symmetry, which has been left exact, comes back in form of the gauge field  $A_\mu$ , defined exactly as in the spinon case in eq. 4.27 and “connecting” the holon and spinon actions which would be otherwise fully independent from each other.

## 4.8 Symmetries of the total effective action for the $t/J$ model

The total effective action for the system  $S(z_\alpha, z_\alpha^*, \Psi_r, \bar{\Psi}_r, A_\mu)$  can be simply obtained by summing 4.26 and 4.34 as:

$$S = \int_0^\beta d\tau \int d^2x \frac{1}{g} \left[ |(\partial_0 - iA_0) z_\alpha|^2 - v_s^2 |(\partial_\mu - iA_\mu) z_\alpha|^2 + m_s^2 (\delta) z_\alpha^* z_\alpha \right] + \sum_{r=1}^2 \bar{\Psi}_r [\gamma_0 (\partial_0 - \delta - e_r A_0) + v_F \gamma_\mu (\partial_\mu - e_r A_\mu)] \Psi_r \quad (4.35)$$

It is to be noted that the original  $U(1)_{h/s} \times U(1)_B \times SU(2)_V$  invariance group has been depleted by the gauge fixing procedure, resulting in just  $U(1)_{h/s}$  remaining. As already noted this local  $U(1)$  gauge invariance is expressed by the gauge field  $A_\mu$ , and, explicitly, corresponds to the following transformations:

$$\left\{ \begin{array}{l} \Psi_r(x) \longrightarrow e^{ie_r \Lambda(x)} \Psi_r(x) \\ \bar{\Psi}_r(x) \longrightarrow e^{-ie_r \Lambda(x)} \bar{\Psi}_r(x) \\ z_\alpha(x) \longrightarrow e^{i\Lambda(x)} z_\alpha(x) \\ z_\alpha^*(x) \longrightarrow e^{-i\Lambda(x)} z_\alpha^*(x) \\ A_\mu(x) \longrightarrow A_\mu(x) - \partial_\mu \Lambda(x) \end{array} \right. \quad \Lambda(x) \in [0, 2\pi[$$

which, as can easily be verified, leave the total effective action in eq. 4.35 invariant. We also note that if one were to neglect the  $A_\mu$  gauge field in eq. 4.35, the dynamics of spinons and holons would be completely independent; the gauge field  $A_\mu$  is effectively a “gauge glue” between the holon and spinon sectors.



# Chapter 5

## Holon pairing

### 5.1 Free holons

In order to analyze the holon pairing the free theory will be analyzed at first, introducing the interaction term at a later stage. The physics of free holons is described by eq. 4.28; here the modulus of  $\hat{\chi}_{ij}^s$  appearing in the hopping term:

$$t \sum_{\langle ij \rangle} \left( H_j^* e^{i \int_{\langle ij \rangle} \bar{B}} H_i \hat{\chi}_{ij}^s + h.c. \right)$$

can be considered as constant, as shown by eq. 4.31, allowing one to approximately rewrite the AM factor as  $\hat{\chi}_{ij}^s = \left| \hat{\chi}_{ij}^s \right| e^{i\theta_{ij}} \sim c \cdot e^{i\theta_{ij}}$ ; however the phase brings a non-negligible spinon contribution to the holon dynamics, and it is only temporarily neglected to be approximately reintroduced at a later time by Peierls substitution. Again, this contribution is due to the  $h/s$  symmetry effectively “binding” holons and spinons.

Under these assumptions, and by noting that the  $\bar{B}$  has no dynamics, only providing a static  $\pi$ -flux phase, one can study holon pairing. In order to do so it is convenient to decompose the lattice in two Néel sublattices,  $A$  with even parity, and  $B$  with odd parity, as already done in the previous

chapter. In the Hamiltonian formalism, the physics described by eq. 4.28 can be conveniently recast as:

$$H_0^h = -t \sum_{i \in A, r=1,4} \left[ e^{i\frac{\pi}{4}(-1)^{r+1}} A_i^\dagger B_{i+r} + h.c. \right] - \mu \sum_{i \in A} A_i^\dagger A_i - \mu \sum_{i \in B} B_i^\dagger B_i$$

with  $r = (\hat{e}_x, \hat{e}_y, -\hat{e}_x, -\hat{e}_y)$ , the  $A_i$  and  $B_i$  fields operators being defined on the sublattices introduced above. It is worth noting that the phase factors, chosen to reproduce the  $\pi$ -flux, can be interpreted as a hopping term  $e^{\pm i\frac{\pi}{4}}$  between different Néel sublattices. When Fourier-transforming these fields operators, it turns out that they are defined on the magnetic Brillouin zone, rather than on the standard Brillouin zone. This diamond-shaped magnetic Brillouin zone (MBZ), as shown in fig. 5.1 is half as big than the standard Brillouin zone, because in position space each  $A$  and  $B$  operator is defined on a  $2a \times a$  lattice.

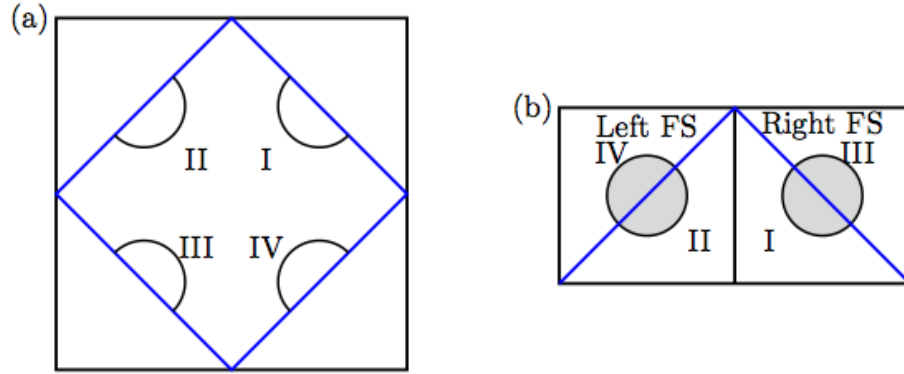


Figure 5.1: From the diamond-shaped magnetic Brillouin zone (a) one can build the rectangular zone (b) by “cut and pasting”, i.e. redefining the operators defined on the MBZ to operate on the rectangular zone. Each half of the rectangular zone can be analyzed separately by assigning a L/R flavour index.

Conveniently the Fourier-transformed operators  $A_{\mathbf{k}}$  and  $B_{\mathbf{k}}$  can be rede-

defined to operate on a rectangular zone equivalent to the MBZ. The rectangular zone can be generated with roto-translations of the third and fourth quadrants, and the operators defined on this new domain will have, with respect to the ones operating on the MBZ, at most a change of sign due to the symmetries of the system; the reader is referred to fig. 5.1 Having defined  $\mathbf{Q}_\pm \equiv (\pm\pi, \pi)$  one can define the following new field operators<sup>1</sup>:

$$a_{\mathbf{k}} = \begin{cases} A_{\mathbf{k}-\mathbf{Q}_+} & \text{if } k_x - \pi < 0, k_y - \pi < 0 \\ A_{\mathbf{k}-\mathbf{Q}_+} & \text{if } k_x + \pi < 0, k_y - \pi < 0 \\ A_{\mathbf{k}} & \text{if } k_y \geq 0 \end{cases}$$

$$b_{\mathbf{k}} = \begin{cases} -B_{\mathbf{k}-\mathbf{Q}_+} & \text{if } k_x - \pi < 0, k_y - \pi < 0 \\ -B_{\mathbf{k}-\mathbf{Q}_+} & \text{if } k_x + \pi < 0, k_y - \pi < 0 \\ B_{\mathbf{k}} & \text{if } k_y \geq 0 \end{cases}$$

and the Hamiltonian for free holons can be written as:

$$\hat{H}_0^h = \sum_{\mathbf{k}} \left( t_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + h.c. \right) - \mu \sum_{\mathbf{k}} \left( \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \right)$$

with  $t_{\mathbf{k}} = 2t \left( \cos(k_x) e^{i\frac{\pi}{4}} + \cos(k_y) e^{-i\frac{\pi}{4}} \right)$ . In order to derive the dispersion relation for free holons one may note that the Hamiltonian above can be recast in the following form:

$$\hat{H}_0^h = \sum_{\mathbf{k}} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \end{pmatrix}^\dagger \begin{pmatrix} \omega - \mu & t_{\mathbf{k}}^* \\ t_{\mathbf{k}} & \omega - \mu \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \end{pmatrix}$$

which immediately gives the dispersion relation for free holons:

$$\epsilon(\mathbf{k}) = \pm |t_{\mathbf{k}}| - \mu = \pm t \sqrt{\cos^2(k_x) + \cos^2(k_y)} - \mu$$

---

<sup>1</sup>Notation: lowercase operators are defined on the rectangular zone, uppercase operators are defined on the original magnetic Brillouin zone.

from which one can see that the Fermi surface for free holons consists of half-circles centered in the four nodal points  $(\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$  in the original diamond-shaped magnetic Brillouin zone.

We can now further modify the domain of the field operators, by noting that the rectangular zone can be divided according to the sign of  $k_x$  in two sub-zones; a flavour  $L$  ( $R$ ) can be assigned to holons respectively in the  $k_x < 0$  ( $k_x \geq 0$ ) sub-zones. This “decomposition” is always exact as long as we deal with non-interacting holons; when introducing an interaction term one will have to demonstrate that the two flavours still do not mix. One is then allowed to redefine once again the domain of the field operators to half of the rectangular zone, i.e.  $[-\frac{\pi}{2}, \frac{\pi}{2}] \times [-\frac{\pi}{2}, \frac{\pi}{2}]$ , provided that a flavour index is introduced. With respect to the rectangular zone the momentum is now measured from  $\mathbf{Q}_R \equiv \frac{1}{2}\mathbf{Q}_+$  in the  $R$  zone, and from  $\mathbf{Q}_L \equiv \frac{1}{2}\mathbf{Q}_-$  in the  $L$  zone, see fig. 5.1. After a final gauge transformation:

$$\begin{cases} a_{\alpha,\mathbf{k}} \longrightarrow a_{\alpha,\mathbf{k}} e^{i\frac{\theta_{\alpha,\mathbf{k}}}{2}} \\ b_{\alpha,\mathbf{k}} \longrightarrow b_{\alpha,\mathbf{k}} e^{-i\frac{\theta_{\alpha,\mathbf{k}}}{2}} \end{cases}$$

with  $\theta_{\alpha,\mathbf{k}} \equiv (-1)^\alpha \left[ \frac{\pi}{4} - \arctan\left(\frac{k_x}{k_y}\right) \right]$  chosen to cancel out a phase factor, the Hamiltonian can be recast in the following form:

$$H_0^h = H_{0,R}^h + H_{0,L}^h = \sum_{\alpha,\mathbf{k} \in D} \left[ v_F |\mathbf{k}| \left( a_{\alpha,\mathbf{k}}^\dagger b_{\alpha,\mathbf{k}} + h.c. \right) - \mu \left( a_{\alpha,\mathbf{k}}^\dagger a_{\alpha,\mathbf{k}} b_{\alpha,\mathbf{k}}^\dagger b_{\alpha,\mathbf{k}} \right) \right] \quad (5.1)$$

$$\text{with } \alpha = R, L, v_F = 2t, D = \left\{ \mathbf{k} \mid -\frac{\pi}{2} < k_x \leq -\frac{\pi}{2}, -\frac{\pi}{2} < k_y \leq -\frac{\pi}{2} \right\}$$

## 5.2 The interaction term and pairing

Let us now introduce the four-holon interaction term, which will provide the attractive interaction needed for holon pairing. It can be read in the third term of the effective hamiltonian for the system (eq. 4.30):



$$\frac{J}{2} \sum_{\langle i,j \rangle} \left( 1 - \hat{h}_i^\dagger \hat{h}_i - \hat{h}_j^\dagger \hat{h}_j \right) \hat{\Delta}_{ij}^s \hat{\Delta}_{ij}^{s\dagger}$$

by expanding the RVB factors to the first order<sup>2</sup> and taking the spatial average of the resulting  $V_\mu^2$  factor one gets an interaction term which reads:

$$\tilde{J} \langle z^\dagger z \rangle \sum_{ij} (-1)^{|i|+|j|} \Delta^{-1}(i-j) \hat{h}_i^\dagger \hat{h}_i \hat{h}_j^\dagger \hat{h}_j \quad (5.2)$$

where  $\Delta^{-1}$  is the 2D inverse lattice Laplacian. The fourth term in eq. 4.30 is neglected in the low-doping limit being proportional to  $\delta^2$ . The spinon-related factors can be treated in mean field approximation as follows, calculating them from the free spinon spectrum:

$$\tilde{J} \langle z^\dagger z \rangle = \int d^2q \frac{1}{\sqrt{|\mathbf{q}|^2 + m_s^2}} = \tilde{J} \left( \sqrt{\Lambda^2 + m_s^2} - m_s \right) \equiv J_{\text{eff}}$$

so that the interaction term which now reads  $J_{\text{eff}} \sum_{ij} (-1)^{|i|+|j|} \Delta^{-1}(i-j) \hat{h}_i^\dagger \hat{h}_i \hat{h}_j^\dagger \hat{h}_j$  and is effectively the one of a 2D Coulomb gas, with particles centered on each holon site, having +1 (-1) charge for being respectively on an even (odd) lattice site. As opposed to all other terms in the theory, it is worth noting that this is a long range interaction term, because  $i$  and  $j$  not being constrained to be nearest neighbours. One should remember that this term is a consequence of the series expansion of a term of the form  $e^{i \int_{\langle ij \rangle} V}$  appearing in the original action, so that it can be observed, as the  $V_\mu$  field describes the  $SU(2)$  vortices centered at each holon site, that the holon attraction is indirect and mediated by the vortices dressing each holon, as shown in fig. 5.2. In our theory this is the driving force for holon pair.

By using known results for the 2D Coulomb gas one can now estimate the pairing temperature for holons, which is given approximately by:

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<sup>2</sup>The expansion is done taking the lattice constant  $a$  as a parameter, so that is possible to truncate consistently the Taylor-expansion after order 1.

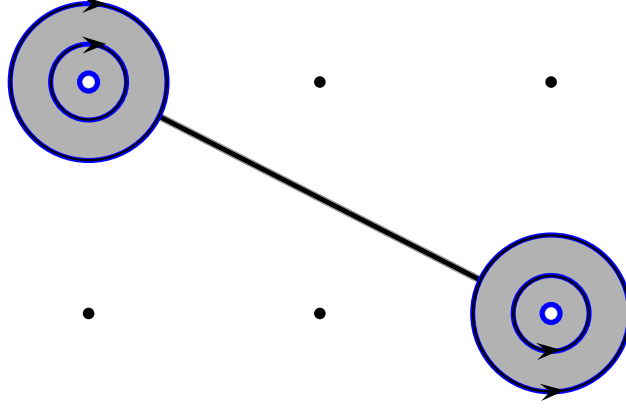


Figure 5.2: The long-range attraction between holons on different sublattices is due to the  $SU(2)$  vortices with opposite chirality surrounding each holon site.

$$T_{ph} \approx \frac{J_{eff}}{2\pi}$$

and the interaction potential in momentum space in the large scale limit will take the following form:

$$V_{eff}(\mathbf{p}) = \frac{J_{eff}}{|\mathbf{p}|^2 + \ell_s^{-2}} \quad (5.3)$$

so that the interaction term is now given in momentum space by:

$$H_I^h \sim - \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}_1, \mathbf{q}_2} V_{eff}(\mathbf{q}_1 - \mathbf{q}_2) \times \delta(\mathbf{p}_1 - \mathbf{p}_2 + \mathbf{q}_1 - \mathbf{q}_2) \hat{a}_{\mathbf{p}_1}^\dagger \hat{b}_{\mathbf{q}_1}^\dagger \hat{b}_{\mathbf{q}_2} \hat{a}_{\mathbf{p}_2}$$

the interaction being written using then L/R flavour indices introduced in the previous section, as it can be seen that even in this interacting case the form of  $V_{eff}$  in eq. 5.3 discourages interactions between different flavours.

By standard BCS treatment one can then obtain the mean-field hamiltonian which describes holon pairing, by adding the BCS-like interaction term to eq. 5.1, which yields:

$$H_\alpha^h = H_{0,\alpha}^h + \sum_{\mathbf{k}} \left( \Delta_{\alpha,\mathbf{k}}^h \hat{a}_{\alpha,\mathbf{k}}^\dagger \hat{b}_{\alpha,-\mathbf{k}}^\dagger + h.c. \right)$$

the modulus of the order parameter  $\Delta_{\alpha,\mathbf{k}}^h$  being defined by the gap equation:

$$\Delta_{\alpha,\mathbf{k}}^h = \sum_{\mathbf{q}} V_{eff}(\mathbf{k} - \mathbf{q}) \frac{\Delta_{\alpha,\mathbf{q}}^h}{2\epsilon_{\alpha,\mathbf{q}}} \tanh\left(\frac{\epsilon_{\alpha,\mathbf{q}}}{2T}\right)$$

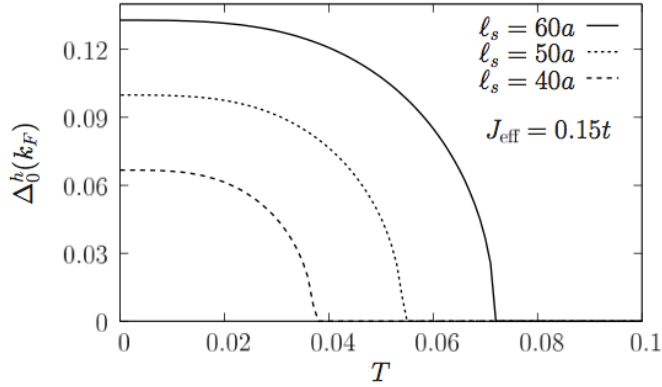


Figure 5.3: Numerical solution for the spinon gap equation, for different values of  $\ell_s$ .

The gap equation can be solved numerically, the results for various screening lengths are shown in fig. 5.3. At last one may want to find the dispersion relation for the interacting holons, in order to do so it is convenient to introduce a four-component spinor field and a  $4 \times 4$  matrix as follows:

$$N_{\alpha,\mathbf{k}} = \begin{pmatrix} a_{\alpha,\mathbf{k}} \\ b_{\alpha,\mathbf{k}} \\ a_{\alpha,-\mathbf{k}}^\dagger \\ b_{\alpha,-\mathbf{k}}^\dagger \end{pmatrix} \quad \mathcal{H}_{\mathbf{k}} = \begin{pmatrix} -\mu & v_F k & 0 & \Delta_{\mathbf{k}}^h \\ v_F k & -\mu & -\Delta_{-\mathbf{k}}^h & 0 \\ 0 & -\Delta_{-\mathbf{k}}^{h*} & \mu & -v_F k \\ \Delta_{\mathbf{k}}^{h*} & 0 & -v_F k & \mu \end{pmatrix}$$

so that the holon pairing Hamiltonian can be recast as:

$$H_{h,\alpha} = \sum_{\mathbf{k}} N_{\alpha,\mathbf{k}}^\dagger \mathcal{H}_{\alpha,\mathbf{k}} N_{\alpha,\mathbf{k}}$$

where  $v_F \equiv 2t$ . Assuming that the order parameter has p-wave symmetry:

$$\Delta_{\mathbf{k}}^h = \begin{cases} \Delta^h(k) \frac{k_x - k_y}{k} & \alpha = R \\ \Delta^h(k) \frac{-k_x - k_y}{k} & \alpha = L \end{cases}$$

$\mathcal{H}_{\mathbf{k}}$  can be block-diagonalized so that the dispersion relation can be written as follows:

$$\epsilon_{\alpha,\mathbf{k}} = \pm \sqrt{(v_F k \pm \mu)^2 + |\Delta_{\alpha,\mathbf{k}}^h|^2} \quad (5.4)$$

It is to be noted that this dispersion relation for interacting holons has four branches: the highest one and the lowest one are completely decoupled and can be neglected in a low-energy description of the system; this assertion is tantamount to saying that of the four components of  $N_{\alpha,\mathbf{k}}$  only two are relevant in the low-energy limit, so that one can describe the theory in terms of the field  $\psi_{\alpha,\mathbf{k}} = \frac{1}{\sqrt{2}}(a_{\alpha,\mathbf{k}} + b_{\alpha,\mathbf{k}})$  and its hermitean conjugate as:

$$H_h = \sum_{\alpha,\mathbf{k}} \begin{pmatrix} \psi_{\alpha,\mathbf{k}} \\ \psi_{\alpha,-\mathbf{k}}^\dagger \end{pmatrix}^\dagger \begin{pmatrix} v_F k - \mu & \Delta_{\alpha,\mathbf{k}}^{h*} \\ \Delta_{\alpha,\mathbf{k}}^h & -v_F k + \mu \end{pmatrix} \begin{pmatrix} \psi_{\alpha,\mathbf{k}} \\ \psi_{\alpha,-\mathbf{k}}^\dagger \end{pmatrix}$$

which allows one to obtain, as expected, the low-energy version of eq. 5.4

$$\epsilon_{\alpha,\mathbf{k}} = \pm \sqrt{(v_F k - \mu)^2 + |\Delta_{\alpha,\mathbf{k}}^h|^2} \quad (5.5)$$

Moreover, recalling the redefinitions of the domain for the field operators and the modifications to the magnetic Brillouin zone which were made when discussing free holons dynamics, one can note that the order parameter is defined on half the rectangular zone and may want to go back to the original

magnetic Brillouin zone. As firstly observed in [34] the p-wave symmetry for the order parameter around each Dirac cone is responsible for a d-wave symmetry in the Brillouin zone; one can explicitly see, indeed, that in the MBZ, in the vicinity of the nodal points  $(\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$  one has:

$$\left\{ \begin{array}{ll} \Delta_{\mathbf{k}}^h \approx v_{\Delta} \frac{k_x - k_y}{\sqrt{2}} & \text{in quadrant I} \\ \Delta_{\mathbf{k}}^h \approx v_{\Delta} \frac{-k_x - k_y}{\sqrt{2}} & \text{in quadrant II} \\ \Delta_{\mathbf{k}}^h \approx v_{\Delta} \frac{-k_x + k_y}{\sqrt{2}} & \text{in quadrant III} \\ \Delta_{\mathbf{k}}^h \approx v_{\Delta} \frac{k_x + k_y}{\sqrt{2}} & \text{in quadrant IV} \end{array} \right.$$

with explicit d-wave symmetry, having defined  $v_{\Delta} = \sqrt{2} \frac{\Delta_0^h(k_F)}{k_F}$ ,  $\Delta_0^h = |\Delta^h|$  and a new coordinate system centered on the nodal points:

$$k_+ \equiv \frac{k_x + k_y}{\sqrt{2}} \quad k_- \equiv \frac{k_x - k_y}{\sqrt{2}}$$

### 5.3 Nodal Hamiltonian and gauge effective action

By noting that the spectrum in eq. 5.5, can also be obtained by the following  $4 \times 4$  matrix, which is again written in terms of the  $\psi_{\mathbf{k}}$  fields introduced in the previous section:

$$\mathcal{H}_{1\text{st},\text{nodal}}^h = v_F k_+ \sigma_z + v_{\Delta} k_- \sigma_y$$

one may think of this theory as an approximation for the full holon Hamiltonian, valid at leading order in the vicinity of nodal points and for low-energy. Restoring the  $h/s$  symmetry by Peierls substitution, and introducing the space-dependent phase for  $v_{\Delta}$  (i.e. a phase for the holon order parameter), one obtains:

$$\mathcal{H}_{1\text{st}}^h = \begin{pmatrix} v_F (-i\partial_+ - A_+) + A_0 & -v_{\Delta} e^{i\phi^h} \partial_- \\ v_{\Delta} e^{-i\phi^h} \partial_- & v_F (i\partial_+ - A_+) - A_0 \end{pmatrix} \quad (5.6)$$

having defined  $\partial_{\pm} \equiv \frac{1}{\sqrt{2}} (\partial_x \pm \partial_y)$ ; the space-dependent phase needs to be reintroduced at this point to maintain the  $\hbar/s$  gauge invariance, however it does not break the nodal structure for holons, justifying the nodal treatment of the present section.  $\mathcal{H}_{1st}^h$  is only valid for the first quadrant, and can be extended to the whole MBZ by repeated rotations. The effective action<sup>3</sup> for this model is a  $QED_3$  action:

$$\mathcal{L}_{1st} = \bar{\chi} [\gamma^{\mu} (\partial_{\mu} - i b_{1st}^{\mu})] \chi$$

having defined  $\gamma^{\mu} = \{\sigma_x, \sigma_y, \sigma_z\}$ ,  $\partial_{\mu} = \{\partial_0, \partial_+, \partial_-\}$ ,  $b_{1st}^{\mu} = \{-ia_+, ia_0, 0\}$ , and having introduced the gauge-invariant nodal fields  $\chi, \bar{\chi} \equiv \chi^{\dagger} \gamma^0$  and  $a_{\mu} \equiv A_{\mu} - \frac{1}{2} \partial_{\mu} \phi^h$ . The action can be integrated as far as the nodon fields are concerned and the leading terms of  $S_{eff}[a_{\mu}] = -\ln \det [\gamma^{\mu} (\partial_{\mu} - i b_{\mu})]$  can be calculated to be:

$$S_{eff}^h[a_{\mu}] = \int d^3k \left( a_0 \Xi_{00} a_0 + \sum_{i=1,2} a_i \Xi_{ii} a_i \right) \quad (5.7)$$

$$\Xi_{00} \sim c_1 \omega \quad \Xi_{ii} \sim c_2$$

for suitable positive constants  $c_1, c_2$ . These terms will be used to introduce, in an approximated way, the holon contribution to spinon pairing in the next chapter.

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<sup>3</sup>Again, only the first quadrant is considered, and again the treatment can easily be extended to the whole MBZ by repeated rotations.

## Chapter 6

# Spinon pairing and superconductivity

### 6.1 Preliminaries

Spinon pairing can be studied by taking into account the four-holon interaction term, i.e. the last term in eq. 4.30. This term has been neglected so far, being proportional to  $\delta^2$  in absence of a finite density of holon pairs; moreover as noted in [7] this term is repulsive for spinons if  $J > 0$ , which is the case, so that the spinon pairing must be mediated by an indirect mechanism. As already anticipated the driving force for spinon pairing is the  $h/s$  gauge interaction, which is indeed attractive and works as outlined in fig. 6.1: as the temperature is lowered each of the two holons in a preformed holon pair becomes able to separately attract a spinon through the  $h/s$  gauge interaction, so that the mechanism ultimately leads to the formation of spinon-RVB pairs,

The aforementioned four-holon interaction term can be rewritten using a Hubbard-Stratonovich transformation to decouple the quartic interaction for spinons, while treating at the same time the holons in MFA, giving rise to the following term:

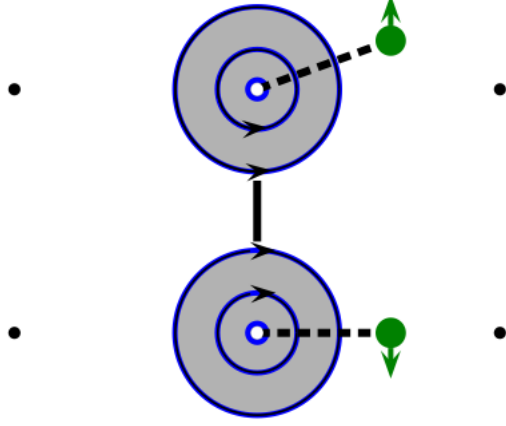


Figure 6.1: The indirect mechanism leading to spinon pairing and to hole pairing; the white dots represent two holons, surrounded by vortices, the solid black line representing the attractive interaction between vortices on different Néel sublattices. The green dots are spinons, with the dashed black lines representing the gauge-mediated holon-spinon interaction.

$$-\sum_{\langle ij \rangle} \frac{2|\Delta_{ij}^s|^2}{J\tau^2} + \Delta_{ij}^{s*} \epsilon^{\alpha\beta} z_{i\alpha} z_{j\beta} + h.c.$$

where  $\tau \equiv \left| \langle \hat{h}_i \hat{h}_j \rangle \right|$  and the spinon order parameter  $\Delta_{ij}^s$  is defined as follows (one must be careful noting that  $\Delta_{ij}^s$  and  $\hat{\Delta}_{ij}^s$  are defined quite differently, not being simply the field and operator version of the same object):

$$\Delta_{ij}^s = \frac{J\tau^2}{2} \langle \epsilon^{\alpha\beta} \hat{z}_{i\alpha} \hat{z}_{j\beta} \rangle$$

Taking the continuum limit, using the exact same procedure which leads to eq. 4.26, the emergent gauge field  $A_\mu \sim z_\beta \partial_\mu z_\beta$  which accounts for the  $h/s$  is again self-generated, and the lagrangian for spinons in real space now reads<sup>1</sup>:

<sup>1</sup>To rewrite the RVB-like factor in the continuum limit one should note that:  $\epsilon^{\alpha\beta} z_{i\alpha} z_{j\beta} = \epsilon^{\alpha\beta} z_{i\alpha} (z_{j\beta} - z_{i\beta}) \rightarrow a \epsilon^{\alpha\beta} z_\alpha \partial_\mu z_\beta = a^2 \left( \epsilon^{\alpha\beta} \frac{z_\alpha \partial_\mu z_\beta}{a} \right)$  having defined  $\mu$  as



$$\mathcal{L}_s = \sum_{\mu=0,1,2} z_\alpha^* [(\partial_\mu - iA_\mu) + m_s^2] z_\alpha + \sum_{i=1,2} \Delta_i^{s*}(\mathbf{x}) \epsilon^{\alpha\beta} z_\alpha \partial_i z_\beta + h.c.$$

with  $\Delta_{ij}^s$ , defined on a lattice link, now being replaced by  $\Delta_i^s(\mathbf{x})$  defined on the continuum with  $i = \{\hat{e}_x, \hat{e}_y\}$  being the spatial direction<sup>2</sup>. Following [7]  $\Delta^s$  can be decomposed separating modulus and phase. The modulus is dependent only on the spatial position, while the phase is dependent only on the direction, so that:

$$\Delta_i^s(\mathbf{x}) = \Delta_{i,0} e^{i\phi^s(\mathbf{x})}$$

We note that the theory is invariant for the  $h/s U(1)$  local gauge symmetry which has been left explicit so far and now takes the form:

$$\begin{cases} z_\alpha \longrightarrow z_\alpha e^{i\Lambda} \\ A_\mu \longrightarrow A_\mu + \partial_\mu \Lambda \\ \phi^s \longrightarrow \phi^s + 2\Lambda \end{cases} \quad \Lambda(\mathbf{x}) \in [0, 2\pi[ \quad (6.1)$$

Also the emergent  $A_\mu$  gauge field “connects” this symmetry to the holon sector, so one may easily convince themselves by looking at eq. 5.6 that in extending the symmetry to the whole system the following transformations must also be added to the ones in eq. 6.1:

$$\begin{cases} H \longrightarrow H e^{i\Lambda} \\ \phi^h \longrightarrow \phi^h + 2\Lambda \end{cases} \quad \Lambda(\mathbf{x}) \in [0, 2\pi[ \quad (6.2)$$

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the direction from the  $i$  site to the  $j$  site.

<sup>2</sup>With respect to eq. 4.26  $g$  and  $v_s$  have been set to 1 for convenience. The other difference lies in the second sum, i.e. the four-holon interaction term opportunely treated, which has been discarded in eq. 4.26 and can no longer be discarded when discussing spinon pairing.

One may want, for the sake of conveniency, to rewrite the theory using  $h/s$  gauge invariant fields; this result may be achieved by defining the following spinon fields:

$$\tilde{z}_1 \equiv z_1 e^{i\phi^s} \quad \tilde{z}_2 \equiv z_2^* e^{-i\phi^s}$$

and the following gauge/phase fields:

$$a_\mu \equiv A_\mu - \frac{1}{2} \partial_\mu \phi^h \quad \phi \equiv \phi^h - \phi^s \quad (6.3)$$

It is readily seen that all these objects are gauge invariant for the  $U(1)$   $h/s$  gauge group and that the Lagrangian for the system, after having defined the doublet  $Z = (\tilde{z}_1, \tilde{z}_2)^T$ , can be rewritten as:

$$\mathcal{L}_s = Z^\dagger(\mathbf{x}) \Gamma_s(\mathbf{x}) Z(\mathbf{x}) \quad (6.4)$$

where the  $2 \times 2$  matrix  $\Gamma_s$  is defined by<sup>3</sup>:

$$\Gamma_s = \sum_{\mu=0,1,2} \left[ \partial_\mu - i \left( a_\mu - \frac{1}{2} \partial_\mu \phi \right) \sigma_z - i \operatorname{Im}(\Delta_{\mu,0}^s) \sigma_x - i \operatorname{Re}(\Delta_{\mu,0}^s) \sigma_y \right]^2 + m_s^2 - |\Delta_{\mu,0}^s|^2 \quad (6.5)$$

By neglecting the gauge fluctuations, one can derive the dispersion relation for spinons by imposing  $\det(\Gamma_s)|_{a_\mu=0, \phi=0} = 0$ . In momentum space one gets:

$$\begin{aligned} 0 &= \left( (-ik_\mu)^2 + m_s^2 \right)^2 + 4 \sum_{\mu,\nu} \Delta_{\mu,0}^s \Delta_{\nu,0}^{s*} (-ik_\mu) (-ik_\nu) = \dots \\ &\dots = \left( (-ik_\mu)^2 + m_s^2 \right)^2 - 4 \sum_{\mu,\nu} \Delta_{\mu,0}^s \Delta_{\nu,0}^{s*} k_\mu k_\nu \end{aligned}$$

from which it is immediate finding an implicate form for the dispersion relation  $\left( -\omega^2 + |\mathbf{k}|^2 + m_s^2 \right)^2 - 4 \sum_{i,j=1,2} \Delta_{i,0}^s \Delta_{j,0}^{s*} k_i k_j = 0$ . By using rotational

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<sup>3</sup>The time component of  $\Delta_{\mu,0}^s$  is defined as zero, i.e.  $\Delta_{\mu,0}^s \equiv (0, \Delta_{i,0}^s)$

invariance for the system, which implies  $\Delta_{i,0}^s \Delta_{j,0}^{s*} + \Delta_{i,0}^{s*} \Delta_{j,0}^s = 2\delta_{ij} |\Delta_{i,0}^s|^2$  one can choose  $\Delta_{1,0}^s = \Delta_0^s$  and  $\Delta_{2,0}^s = i\Delta_0^s$  for a constant complex number  $\Delta_0^s$ . Solving for  $\omega$  one readily obtains the dispersion relation:

$$E_{\pm}(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m_s^2 \pm 2|\Delta_0^s| |\mathbf{k}|} \quad (6.6)$$

The two branches of the dispersion relation, the lower showing quite a peculiar minimum, are shown in fig. 6.2.

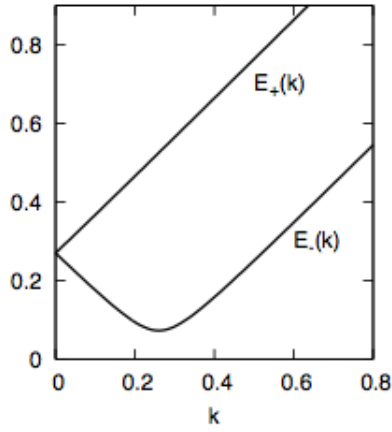


Figure 6.2: Spinon spectrum for  $\delta = 0.1$ .

## 6.2 Gauge effective action for spinons

It is convenient to recast eq. 6.4 by introducing a fictitious  $SU(2)$  gauge field  $Y_\mu$ . The matrix  $\Gamma_s$  can be equivalently written as:

$$\Gamma_s = \sum_{\mu=0,1,2} \left( \partial_\mu - iY_\mu^a \frac{\sigma_a}{2} \right)^2 + M^2$$

provided that the fictitious mass  $M$  is defined as  $M \equiv \sqrt{m_s^2 - 2|\Delta_0^s|^2}$  and the fictitious gauge field is defined as:

$$Y_\mu^a = \begin{pmatrix} 0 & 0 & a_0 + \partial_0 \phi \\ \text{Im}(\Delta_{1,0}^s) & \text{Re}(\Delta_{1,0}^s) & a_1 + \frac{1}{2} \partial_1 \phi \\ \text{Im}(\Delta_{2,0}^s) & \text{Re}(\Delta_{2,0}^s) & a_2 + \frac{1}{2} \partial_2 \phi \end{pmatrix}$$

One can then integrate out the spinon fields in eq. 6.4 and obtain an effective action written only in terms of the gauge field  $a_\mu$ , the modulus of the order parameter  $\Delta_0^s$  and the derivative of the electron phase  $\partial_\mu \phi$ :

$$S_{eff}^s [a_\mu, \Delta_0^s, \partial_\mu \phi] = \ln \det (\Gamma_s) - \frac{2 |\Delta_0^s|^2}{J\tau^2} \quad (6.7)$$

One can then Taylor-expand  $S_{eff}^s$ :

$$S_{eff}^s \approx S_{eff}^{s,0} [0, 0, \Delta_s] + S_{eff}^{s,2} [\partial_\mu \phi, a_\mu, \Delta_s] + \dots \quad (6.8)$$

The action can then be written as a Taylor expansion in the number of fields; the zeroth order term can simply be found by setting  $a_\mu = 0 = \partial_\mu \phi$ . The higher-order terms actually are highly constrained by gauge and rotational invariances: it can be easily seen that no first order terms satisfies these requests and that the only acceptable second order term is (proportional to)  $\text{tr} [f_{\mu\nu} f^{\mu\nu}] + \text{const}$ ,  $f_{\mu\nu}$  being the field strength for  $Y_\mu$ . The two terms are derived as follows:

- The former can be obtained by simply setting  $a_\mu$  and  $\phi$  to zero in the fictitious gauge field  $Y_\mu$ , so that:

$$Y_\mu^a = 2 \begin{pmatrix} 0 & 0 & 0 \\ \text{Im}(\Delta_{2,0}^s) & \text{Re}(\Delta_{1,0}^s) & 0 \\ \text{Im}(\Delta_{2,0}^s) & \text{Re}(\Delta_0^s) & 0 \end{pmatrix}$$

and taking the determinant in momentum space:

$$S_{eff}^{s,0} = \sum_k \ln \det \left[ \left( k_\mu - Y_\mu^a \frac{\sigma_a}{2} \right)^2 + M^2 \right] =$$

$$\begin{aligned}
&= \sum_{\omega, \mathbf{k}} \ln \left[ \left( \omega^2 + |\mathbf{k}|^2 + M^2 + 2|\Delta_0^s|^2 \right)^2 - 4|\Delta_0^s|^2 |\mathbf{k}|^2 \right] = \\
&= \sum_{\omega, \mathbf{k}} \ln \left[ (\omega^2 + E_-^2(\mathbf{k})) (\omega^2 + E_+^2(\mathbf{k})) \right]
\end{aligned}$$

- As far as the latter term is concerned, it is proportional to the field strength up to an additive constant, i.e. the field strength may not go to zero when the fields go to zero, as one is entitled to expect from a “fluctuations” term. So we start by calculating the field strength:

$$\begin{aligned}
f_{\mu\nu} &= \frac{1}{i} [D_\mu, D_\nu] = -i \left[ \partial_\mu + i\partial_\mu\phi^s - iY_\mu^a \frac{\sigma^a}{2}, \partial_\nu + i\partial_\nu\phi^s - iY_\nu^a \frac{\sigma^a}{2} \right] = \dots \\
&\dots = (\partial_\mu\partial_\nu\phi^s - \partial_\nu\partial_\mu\phi^s) - \frac{\sigma_c}{2} \underbrace{\left[ \partial_\mu Y_\nu^c - \partial_\nu Y_\mu^c + \epsilon^{abc} Y_\mu^a Y_\nu^b \right]}_{\equiv y_{\mu\nu}^a}
\end{aligned}$$

Due to the properties of the Pauli matrices (namely  $\sigma_a^2 = \mathbb{1}$ ) we have:

$$S_{\text{eff}}^{s,2} = \lambda \text{tr} [f_{\mu\nu} f^{\mu\nu}] = \lambda (\partial_\mu\partial_\nu\phi^s - \partial_\nu\partial_\mu\phi^s)^2 + \frac{\lambda}{4} y_{\mu\nu}^a y_{\mu\nu}^a$$

and the last term can be evaluated by using the fact that  $Y_\mu^{x,y}$  is uniform in space:

$$\frac{1}{2} y_{\mu\nu}^a y_{\mu\nu}^a = \left[ 2(\partial_1 a_2 - \partial_2 a_1) + 2(a_0 + \partial_0\phi)^2 + (\mathbf{a} + \nabla\phi)^2 \right] + [\partial_\mu a_\nu - \partial_\nu a_\mu]^2 + |\Delta_0^s|^4$$

Clearly  $|\Delta_0^s|^4$  is the constant term which need to be discarded, by imposing the request  $\text{tr} [f_{\mu\nu} f^{\mu\nu}]|_{a_\mu=0=\phi^s=\phi} = 0$ , however it is useful to set the global multiplicative constant  $\lambda$ , by matching the Taylor-expansion in  $|\Delta_0^s|$  at the fourth order the multiplicative constant turns out to be:  $\lambda = (3\pi M)^{-1}$ .

To sum up, spinon pairing can be studied by Taylor-expanding the effective action in eq. 6.7 in the number of fields. An expansion up to the second order is able to include gauge fluctuations, so that the spinon pairing is correctly reproduced; the first two terms of the expansion are<sup>4</sup>:

$$S_{\text{eff}}^{s,0} = -\frac{2|\Delta_0^s|^2}{J\tau^2} + \sum_{\omega, \mathbf{k}} \ln [(\omega^2 + E_-^2(\mathbf{k})) (\omega^2 + E_+^2(\mathbf{k}))] \quad (6.9)$$

$$S_{\text{eff}}^{s,2} = \frac{1}{6\pi M} \left\{ [\partial_\mu a_\nu - \partial_\nu a_\mu]^2 + |\Delta_0^s|^2 \left[ 2 \left( a_0 + \frac{1}{2} \partial_0 \phi \right)^2 + \left( \mathbf{a} + \frac{1}{2} \nabla \phi \right)^2 \right] \right\} \quad (6.10)$$

The latter term is a three-dimensional anisotropic gauged XY model and, as we will see, plays a key role in determining the superconducting transition. Here we remind that the 3D XY model, to which 6.10 is essentially equivalent under appropriate assumptions which will be discussed and demonstrated later, shows two phases:

- For large enough temperature (or for small enough  $|\Delta_0^s|^2$ , as  $|\Delta_0^s|$  is monotonically decreasing function of temperature) the model is in a vortex-antivortex<sup>5</sup> proliferation state; the phase fluctuate strongly and, as a result,  $\langle e^{i\phi} \rangle = 0$ . We will refer to this phase as the Coulomb phase.
- For small enough temperature the creation of a new vortex-antivortex pair is no longer energetically favorable; the fluctuations for the  $\phi$  field are exponentially suppressed so that  $\langle e^{i\phi} \rangle \neq 0$  and, finally, SC onsets. We will refer to this phase as the broken symmetry phase, also called Higgs phase.

<sup>4</sup>An irrelevant surface term has been discarded in  $S_{\text{eff}}^{s,2}$ .

<sup>5</sup>Being this a 3D model one should rigorously speak of “vortex lines” and “antivortex lines”

### 6.3 Gap equation for spinons

As noted, the direct interaction between spinons is repulsive; so that the pairing must be described by also taking into account the gauge fluctuations, namely the term  $S_{eff}^{s,2}$  in eq. 6.8. As discussed in [7] and citations therein, the correct procedure to get the gap equation is starting from the partition function while neglecting the phase fluctuations; i.e. one wants to find the saddle point point of  $S_{eff}^s[a, \Delta_0^s] = S_{eff}^{s,0}[\Delta_0^s] + S_{eff}^{s,2}[a, \Delta_0^s] + S_{eff}^h[a]$  where  $S_h$  is the contribution from the holon sector, namely from eq. 5.7. The aim of this section is to calculate the free energy for the system, from which the gap equation can be calculated; it is clearly seen that the contribution to the free energy from  $S_{eff}^{s,0}[\Delta_0^s]$  is readily calculated. On the other hand the contribution for  $S_{eff}^{s,2} + S_h$  involves a calculation which will now be carried out; we will refer to this contribution as the “gauge” contribution to free energy. The gauge partition function is then<sup>6</sup>:

$$Z_g = \int \mathcal{D}a_\mu e^{-\int d^3x \mathcal{L}_g[a_\mu]} \quad \mathcal{L}_g = \frac{1}{3\pi M} [a_\mu (-\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu + m^{\mu\nu}) a_\nu]$$

with the following “pseudo-mass” matrix:

$$m^{\mu\nu} = \begin{pmatrix} |\Delta_0^s|^2 + \tilde{c}_2 & 0 & 0 \\ 0 & \frac{|\Delta_0^s|^2}{2} + f(\mathbf{k}) & 0 \\ 0 & 0 & \frac{|\Delta_0^s|^2}{2} + f(\mathbf{k}) \end{pmatrix} \quad (6.11)$$

The holon contribution is clearly included in  $\tilde{c}_2 = 3\pi M c_2$  and in  $f(\mathbf{k}) = 3\pi M c_1 \sqrt{v_F^2 k_+^2 + v_\Delta^2 k_-^2}$ , which are taken from 5.7. It is now convenient using the transformation in 6.3 for the gauge field  $a_\mu$ , which along with the gauge transformations in eq. 6.1 and 6.2, allows one to rewrite the gauge partition function  $Z_g$  and the lagrangian  $\mathcal{L}_g$  as follows:

<sup>6</sup>Using the usual Euclidean metric  $g^{\mu\nu} = \text{diag}(1, 1, 1)$

$$\begin{aligned}\mathcal{L}_g &= \frac{1}{3\pi M} A_\mu (-\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu + m^{\mu\nu}) A_\nu - \frac{1}{4} \phi^h \partial_\mu m^{\mu\nu} \partial_\nu \phi^h + \phi^h m^{\mu\nu} \partial_\mu A_\nu \\ Z_g &= \int \mathcal{D}A_\mu \mathcal{D}\phi^h e^{-\int d^3x \mathcal{L}_g}\end{aligned}\tag{6.12}$$

The gauge partition function in eq. 6.12 clearly needs the gauge to be fixed, as the  $h/s$  symmetry has been kept exact up to this point. A convenient choice of the gauge fixing function is  $F = -m^{\mu\nu} \partial_\mu A_\nu + \frac{1}{2} \phi^h$ , which allows one to decouple the  $A_\mu$  and  $\phi^h$  terms so that the functional can be evaluated integral after having completed the Faddeev-Popov gauge-fixing procedure:

$$Z_g = \int \mathcal{D}A_\mu \mathcal{D}\phi^h \left| \frac{\delta F}{\delta \Lambda} \right| e^{-\int d^3x \frac{1}{3\pi M} (A_\mu K^{\mu\nu} A_\nu + \frac{1}{4} \phi^h D \phi^h)}\tag{6.13}$$

where  $K^{\mu\nu}$  and  $D$  are defined as follows:

$$\begin{aligned}K^{\mu\nu} &= -\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu + m^{\mu\nu} - m^{\mu\mu'} m^{\nu\nu'} \partial_{\mu'} \partial_{\nu'} \\ D &= -m^{\mu\nu} \partial_\mu \partial_\nu + 1\end{aligned}$$

The result of the functional integral is then:

$$Z_g = \prod_{\omega, \mathbf{k}} \frac{(3\pi M)^{\frac{3}{2}}}{\left(\omega^2 + |\mathbf{k}|^2 + m^{11}\right)^{\frac{1}{2}} \left(\omega^2 + \frac{m^{11}}{m^{00}} |\mathbf{k}|^2 + m^{11}\right)^{\frac{1}{2}}}\tag{6.14}$$

It is now straightforward to get the free energy  $F_g$ , summing the contribution from eq. 6.14 and the contribution from  $S_{\text{eff}}^{s,0}$ :

$$\frac{1}{V} F_g [\Delta_0^s] \approx \frac{1}{\beta V} \sum_{\omega, \mathbf{k}, \sigma=\pm} \ln(\omega^2 + E_\sigma^2(\mathbf{k})) - \frac{3\Lambda^3}{4} \left[ \ln m_s^2 - \frac{2|\Delta_0^s|^2}{m_s^2} \right] - \Lambda^2 \frac{|\Delta_0^s|^2}{J\tau^2}$$

and the gap equation, by deriving the free energy  $F_g$  with respect to  $|\Delta_0^s|$ :



$$0 = \frac{2\Lambda}{3m_s^2} - \frac{\Lambda^2}{J\tau^2} - \frac{1}{2|\Delta_0^s|V} \sum_{\mathbf{k}} \left[ \frac{|\mathbf{k}|}{E_-(\mathbf{k}) \tanh\left(\frac{E_-(\mathbf{k})}{2T}\right)} - \frac{|\mathbf{k}|}{E_+(\mathbf{k}) \tanh\left(\frac{E_+(\mathbf{k})}{2T}\right)} \right] \quad (6.15)$$

Some numerical solutions for the gap equation for spinons, at different dopings, are shown in fig. 6.3, the physical meaning of the gap and its role in the onset of superconductivity will be discussed in the following section.

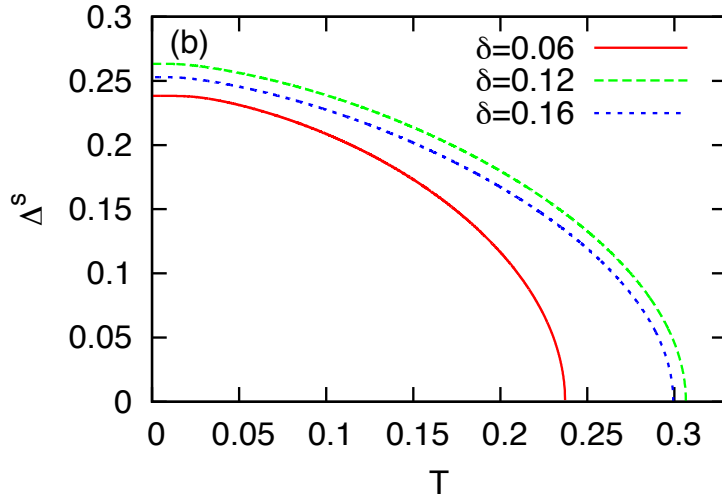


Figure 6.3: The numerical solution for the gap equation for spinons in eq. 6.15, for various doping values.

Finally we can identify the line corresponding to  $T_{ps}$  at various dopings in the  $T - \delta$  phase diagram, by solving eq. 6.15 for the temperature at various dopings, having imposed  $|\Delta_0^s| = 0$ ; the aforementioned line is the one labelled with  $\Delta^s = 0.0$  in fig. 6.4.

## 6.4 Superconductivity

The order parameter for superconductivity is to be written, in terms of  $c_i$ ,  $c_i^\dagger$ , i.e. electron annihilation/creation operators, as:

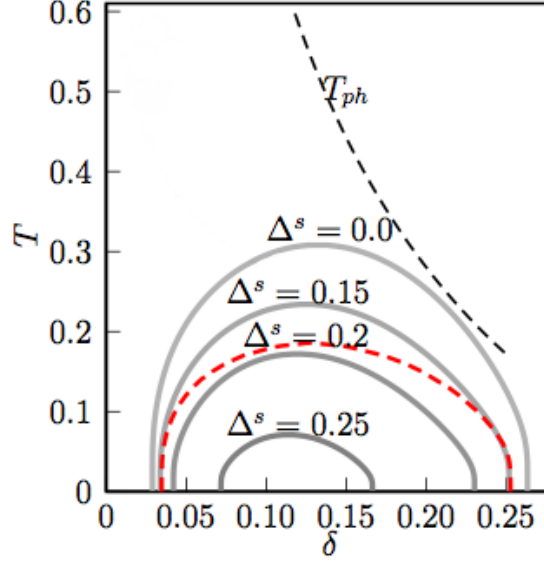


Figure 6.4: Phase diagram, the line labelled with  $\Delta^s = 0.0$  is the one which marks  $T_{ps}$ .

$$\Delta_{ij}^c = \langle \epsilon^{\alpha\beta} c_{i\alpha} c_{j\beta} \rangle$$

by consistently neglecting gauge fluctuations, in accordance with eq. 4.19 and eq. 4.20, it can be rewritten in terms of spinonic and holonic operators as:

$$\Delta_{ij}^c = \langle \epsilon^{\alpha\beta} z_{i\alpha} z_{j\beta} \rangle \langle H_i^* H_j^* \rangle$$

so that in term of  $\Delta_0^h$ ,  $\Delta_0^s$  and their respective phases, as defined when discussing holon and spinon pairing, the order parameter for superconductivity is then defined as:

$$\Delta_c \sim \frac{\Delta^s}{\Delta^h} = \frac{\Delta_0^s}{\Delta_0^h} e^{i(\phi^h - \phi^s)}$$

For the onset of SC the condition  $\langle \Delta_c \rangle \neq 0$  must be fulfilled. Namely a finite density of holons and spinons should be present in the system (i.e.

$\langle \Delta_0^s \rangle \neq 0$  and  $\langle \Delta_0^h \rangle \neq 0$ ) but also the gauge-invariant electron phase  $\phi = \phi^h - \phi^s$  should condense, i.e.  $\langle e^{i\phi} \rangle \neq 0$ , not to destroy superconductivity. Equivalently one may say that the superconductivity is achieved in three steps:

- At first a finite density of incoherent holon pairs is formed at a temperature  $T_{ph}$ . As seen the attractive force allowing holon to pair is given by spin vortices surrounding each holon site.
- A finite density of incoherent spinon pairs is formed at an intermediate temperature  $T_{ps}$ . As seen, there is no “direct” attraction between spinons; however as each of the two holons in a preformed holon pair is able of attracting a spinon by means of the  $h/s$  gauge interaction, this whole mechanism can be regarded in its entirety as an effective attractive interaction between spinons, mediated by the  $A_\mu$  gauge field and a preformed holon pair. In this regime the superconductivity is destroyed by a plasma of magnetic vortices-antivortices, described by the gradient of the phase  $\phi$  which is oscillating too strongly for superconductivity to appear. It has been argued ([7]) that this regime corresponds to the appearance of the Nerst signal<sup>7</sup> above the SC dome. We also note that  $T_{ps}$  must be  $\leq T_{ph}$  because the whole treatment of holon pairing assumes  $\tau \equiv \left| \langle \hat{h}_i \hat{h}_j \rangle \right| \neq 0$ ; indeed, the gap equation has no solution if  $\tau = 0$  so that there can be no spinon pairing in absence of holon pairing.
- Finally at a temperature  $T_c$  the preformed holes became coherent, generating a d-wave hole condensate:

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<sup>7</sup>The Nerst signal is observed as an electric field generated when a sample is subjected to a temperature gradient and a magnetic field, perpendicular to each other. The electric field generated as a response is perpendicular to both.

$$\langle \sum_{\alpha, \beta} \epsilon^{\alpha\beta} c_{i\alpha} c_{j\beta} \rangle \neq 0$$

This transition corresponds to the condensation of the phase field, in other words  $T_c$  is determined by the condition  $\langle e^{i\phi} \rangle \neq 0$ ; the dynamics of the  $\phi$  field, as seen, are essentially those of a three-dimensional XY model, so that it can be argued that the superconducting transition is in the 3DXY universality class; this remarked will be explained more thoroughly when discussing the behaviour of the superfluid density in the vicinity of  $T_c$ . Below  $T_c$  the  $U(1)$  symmetry for the  $h/s$  gauge field is broken to the  $\mathbb{Z}_2$  discrete group, implying, due to the Anderson-Higgs mechanism, that the gauge field  $A_\mu$  should acquire mass. It has been proved<sup>8</sup> that the coherence for holon pairing is inconsistent with a gapless  $A_\mu$  field, so that  $T_c$  must be  $\leq T_c$ .

- It is then now that the superconductivity is ultimately determined by the 3DXY model in eq. 6.10, the superconducting transition being determined by a finite  $|\Delta_0^s|$  which we will denote as  $|\Delta_0^s|_c$ ; i.e. the value which separates the Higgs and Coulomb phases for the 3DXY model. The exact value of this quantity will be calculated in subsection 7.2.2, here we note that, referring to the phase diagram in fig. 6.4, for every choice of  $|\Delta_0^s|_c$  the present theory is able to reproduce the dome-shaped superconducting zone in the  $T - \delta$  phase diagram.

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<sup>8</sup>See Appendix C of [7]

## Chapter 7

# Superfluid density

As previously discussed in section 2.6 the superfluid density has two operative definitions which yield the same result in the context of BCS theory, but do not necessarily agree in the context of other theories for superconductivity. Particularly, as in the framework of the present theory a finite incoherent density of hole pairs is present at  $T_c \leq T \leq T_{ps}$ , in this range of temperatures we expect to have  $\rho_s^{EM} = 0$ , as the gauge field is still ungapped, and  $\rho_s^F \neq 0$ , as the mechanical definition of superfluid density is oblivious of whether the pairs are in a coherent or incoherent state.

The calculations for both  $\rho_s^{EM}$  and  $\rho_s^F$  will be now be carried out, as the original contribution of the present thesis. We start by recalling that, as shown in eq. 6.8, the effective action for the system, when also including holon contribution, reads:

$$S_{\text{eff}}^s[a, \Delta_0^s] = S_{\text{eff}}^{s,0}[\Delta_0^s] + S_{\text{eff}}^{s,2}[a, \Delta_0^s] + S_{\text{eff}}^h[a]$$

and that this action can be interpreted as a zeroth order expansion, i.e.  $S_{\text{eff}}^{s,0}$ , to which the gaussian fluctuations in the gauge fields have been added, by means of  $S_{\text{eff}}^{s+h,2} = S_{\text{eff}}^{s,2}[a, \Delta_0^s] + S_{\text{eff}}^h[a]$ . However  $S_{\text{eff}}^{s,0}$  and  $S_{\text{eff}}^{s+h,2}$  when analyzed separately can be regarded as describing two different theories, giving two different contributions to the superfluid density each one on its own:

- $S_{\text{eff}}^{s,0}$  is formally similar to the action a BCS-like theory<sup>1</sup>. However the analogy cannot be extended as there are striking qualitative differences: as opposed to the BCS case, this term alone does not provide attractive interaction due to the different statistics of the fields involved. In this term one would expect to observe<sup>2</sup>  $\rho_s^F \neq 0$ , while the contribution to  $\rho_s^{EM}$  must be null for at least two reasons: in first place, by definition the phase field fluctuations are not included in this term, so that no coefficient can be identified; also, as noted in [10], to be defined  $\rho_s^{EM}$  requires the existence of long-range topological order. Also this is in full accordance with the fact, already analyzed, that  $S_{\text{eff}}^{s,0}$  alone is not enough to describe superconductivity, the gauge fluctuations being essential in describing the symmetry breaking related to the SC transition: keeping this remark in mind it is natural assuming that in this sector  $\rho_s^{EM}$  should be zero.
- $S_{\text{eff}}^{s,2}$  effectively describes a three-dimensional gauged anisotropic XY model, in which the time component can be treated effectively as a spatial variable and the coefficient  $\frac{|\Delta_0^s|^2}{6\pi M}$  can be regarded as the inverse temperature, determining which phase the model is in. The coefficient is a monotonically decreasing function of temperature, as is the inverse temperature, so that qualitatively the distinction between the high-temperature phase and low-temperature phase of the model is preserved. As already noted, for numerical reasons in a three-dimensional model  $\rho_s^{EM}$  and  $\rho_s^F$  are effectively the same quantity up to a part in  $10^4$ , so that the distinction between the two definitions can be neglected in

<sup>1</sup>Compare for instance our  $2 \times 2$  matrix in eq. 7.4 with its corresponding fermionic BCS analogue in [14]

<sup>2</sup>The physical meaning being that  $S_{\text{eff}}^{s,0}$  describes a finite density of finite holons, provided that the gap equation is solved taking into account the gauge fluctuations so that  $|\Delta_0^s|$  can be  $\neq 0$ . If we restrict ourselves to a pure  $S_{\text{eff}}^{s,0}$  theory clearly we will also observe  $\rho_s^F = 0$ , because, as already noted, the interaction between spinons is repulsive.

this case.

Following the scheme just outlined, the calculation will be split in two parts, separating the contribution to  $\rho_s$  coming from  $S_{\text{eff}}^{s,0}$  from the one coming from  $S_{\text{eff}}^{s+h,2}$ . We will refer to these two contributions as  $\rho_{s,0}$  and  $\rho_{s,2}$ , keeping in mind that for the former is obtained by using the mechanical definition for  $\rho_s$ , while on the other hand for the latter the two definitions are in good agreement.

## 7.1 Calculation of $\rho_{s,0}$

Aim of this section will be calculating the contribution to the superfluid density coming from  $S_{\text{eff}}^{s,0}$ , which, as already noted can only contribute to the “mechanically-defined” superfluid density. The basic idea behind this calculation is that, as stated in eq. 2.13 the “mechanically-defined” superfluid density can be evaluated by calculating the second order free energy difference when imposing a phase twist

$$\Delta_c(x) \longrightarrow \Delta'_c(x) = \Delta_c(x) e^{-i\mathbf{Q}\cdot\mathbf{x}} \quad (7.1)$$

to the SC order parameter. As seen, in our model the SC order parameter is given by:

$$\Delta_c = \frac{\Delta_{s,0}}{\Delta_{h,0}} e^{i\phi} \quad (7.2)$$

and, in order to calculate  $\rho_{s,0}$ , we will be observing how the twist eq. 7.1 modifies the dispersion relation, the partition function and, at last, the free energy for the system, from which the superfluid density can be calculated.

### 7.1.1 The dispersion relation for spinons

Preliminarily we recall that the dispersion relation for the system can be conveniently found starting from the Lagrangian for spinons in the Nambu

spinor representation:

$$\mathcal{L} = \tilde{z}^\dagger(x) \Gamma_s(x) \tilde{z}(x) \quad (7.3)$$

after having opportunely defined a bosonic gauge-neutral Nambu-Gor'kov doublet:

$$\tilde{z} = \begin{pmatrix} \tilde{z}_1 \\ \tilde{z}_1 \end{pmatrix} = \begin{pmatrix} z_1 e^{i\phi/2} \\ z_2 e^{-i\phi/2} \end{pmatrix}$$

with  $\Gamma_s$  as defined in 6.5, which in matrix form reads:

$$\Gamma_s = \begin{pmatrix} (\partial_\mu - i(a_\mu + \frac{1}{2}\partial_\mu\phi))^2 + m_s^2 & -2\Delta_\mu\partial^\mu \\ 2\Delta_\mu^*\partial^\mu & (\partial_\mu + i(a_\mu + \frac{1}{2}\partial_\mu\phi))^2 + m_s^2 \end{pmatrix} \quad (7.4)$$

For the sake of simplicity of notation only throughout the present section we will often drop some unnecessary indices on the spinon order parameter, by defining  $\Delta_\mu \equiv \Delta_{\mu,0}^s$ . By neglecting the gauge and phase fields and taking the determinant of  $\Gamma_s$  in momentum space the two-branch dispersion relation for spinons is found to be  $E_\pm(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m_s^2 \pm 2|\Delta_0^s||\mathbf{k}|}$ , assuming rotational invariance for the system.

Now, in order to be able to evaluate the free energy when imposing the aforementioned twist to the order parameter, we are interesting evaluate how the dispersion relation changes upon the same twist, i.e. carrying out the same calculation as above after having modified the order parameter. More specifically, when deriving the dispersion relation after imposing the twist

$$\Delta(x) \longrightarrow \Delta'(x) = \Delta(x) e^{-i\mathbf{Q}\cdot\mathbf{x}}$$

for an infinitesimal  $\mathbf{Q}$  on the order parameter of the SC  $\Delta_c = \frac{\Delta_0^s}{\Delta_0^h} e^{i\phi}$  it is convenient to include the actual twist in  $\Delta_0^s$ , so that it is no longer a real number, gaining an infinitesimal imaginary component.



The twist then modifies the  $2 \times 2$   $\Gamma_s$  matrix in eq. 6.5 in the following way:<sup>3</sup>:

$$\Gamma_s \longrightarrow \Gamma'_s = \begin{pmatrix} (\partial_\mu - i(a_\mu + \frac{1}{2}\partial_\mu\phi))^2 + m_s^2 & -2e^{-i\mathbf{Q}\cdot\mathbf{x}}\Delta_\mu\partial^\mu \\ 2e^{i\mathbf{Q}\cdot\mathbf{x}}\Delta_\mu^*\partial^\mu & (\partial_\mu + i(a_\mu + \frac{1}{2}\partial_\mu\phi))^2 + m_s^2 \end{pmatrix}$$

It is worth emphasizing, as the notation can be a little misleading at first, that the phase  $\phi = \phi_h - \phi_s$  is left unchanged by this treatment, the only quantity changed being  $\Delta_0^s$ . As a consequence the fields  $a_\mu$  and  $\phi$  are also unchanged.

In order to understand the physics this new  $\Gamma'_s$  matrix describes, it is convenient doing a pseudo-unitary transformation. Normally such a transformation in a fermionic BCS-like theory would be a *unitary* transformation. In the present case, however, a pseudo-unitary transformation is needed (i.e. a transformation  $U$  such that  $U^\dagger\sigma_3U = \sigma_3$ ) because the fields are bosonic, as noted in [14], § 2.2 and in [35]. Nonetheless the transformation used, being diagonal, is both unitary and pseudo-unitary. The basic idea behind this transformation is removing the additional phase that the twist adds to the off-diagonal terms, at the expense of making the on-diagonal terms more complicated. It is worth noting that such a transformation leaves the physics of the system unchanged, as  $S \sim \ln \det(\Gamma_s) = \ln \det(U^{-1}\Gamma_sU)$ <sup>4</sup>. One can then choose the following transformation:

$$U = \begin{pmatrix} e^{-i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} & 0 \\ 0 & e^{+i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} \end{pmatrix} \quad (7.5)$$

after which the  $\Gamma_s$  becomes:

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<sup>3</sup>Generally in the present and in the following section the prime will be used to indicate the quantities after the twist.

<sup>4</sup>This is not completely true, as the UV cutoff forces us to make some additional considerations, see subsection 7.1.3.

$$U^{-1}\Gamma'_s U = \begin{pmatrix} e^{+i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}}\Gamma'_{11}e^{-i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} & e^{+i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}}\Gamma'_{12}e^{+i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} \\ e^{-i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}}\Gamma'_{21}e^{-i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} & e^{-i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}}\Gamma'_{22}e^{+i\frac{\mathbf{Q}\cdot\mathbf{x}}{2}} \end{pmatrix}$$

and letting the differential operators act on the phase factors<sup>5</sup>:

$$U^{-1}\Gamma'_s U = \begin{pmatrix} \left(\partial_\mu - \xi_\mu - i\frac{Q_\mu}{2}\right)^2 + m_s^2 & -2\Delta_\mu \left(\partial^\mu - i\frac{Q_\mu}{2}\right) \\ 2\Delta_\mu^* \left(\partial^\mu + i\frac{Q_\mu}{2}\right) & \left(\partial_\mu + \xi_\mu + i\frac{Q_\mu}{2}\right)^2 + m_s^2 \end{pmatrix}$$

As already done while deriving the dispersion relation in the standard case, we set the gauge and phase fields to zero, and then we calculate the determinant of  $\Gamma_s$  in momentum space:

$$0 = \begin{vmatrix} \left(\partial_\mu - i\frac{Q_\mu}{2}\right)^2 + m_s^2 & -2\Delta_\mu \left(\partial^\mu + i\frac{Q_\mu}{2}\right) \\ 2\Delta_\mu^* \left(\partial^\mu - i\frac{Q_\mu}{2}\right) & \left(\partial_\mu + i\frac{Q_\mu}{2}\right)^2 + m_s^2 \end{vmatrix} \longrightarrow$$

$$\xrightarrow{\text{Fourier}} \left(-\omega^2 + |\mathbf{k}|^2 + m_s^2 + \frac{|\mathbf{Q}|^2}{4}\right)^2 - (\mathbf{k} \cdot \mathbf{Q})^2 - 4 \sum_{i,j=1,2} \Delta_i^* \Delta_j \left(\mathbf{k} + \frac{\mathbf{Q}}{2}\right)_i \left(\mathbf{k} - \frac{\mathbf{Q}}{2}\right)_j = 0$$

We rewrite the sum in a more convenient way, using  $\sum_{i,j} = \sum_{i=j} + \sum_{i \neq j}$  and the rotational invariance of  $\Delta_i$ , which implies  $\Delta_i \Delta_j^* + \Delta_i^* \Delta_j = 2\delta_{ij} |\Delta_i|^2$ :

$$\begin{aligned} & \sum_{i,j=1,2} \Delta_i^* \Delta_j \left(\mathbf{k} + \frac{\mathbf{Q}}{2}\right)_i \left(\mathbf{k} - \frac{\mathbf{Q}}{2}\right)_j = \\ & = \sum_{i=j} \Delta_i^* \Delta_j \left(\mathbf{k} + \frac{\mathbf{Q}}{2}\right)_i \left(\mathbf{k} - \frac{\mathbf{Q}}{2}\right)_j + \sum_{i \neq j} \Delta_i^* \Delta_j \left(\mathbf{k} + \frac{\mathbf{Q}}{2}\right)_i \left(\mathbf{k} - \frac{\mathbf{Q}}{2}\right)_j = \\ & = |\Delta_0^s|^2 \sum_{i=1,2} \left(k_i^2 - \frac{Q_i^2}{4}\right) + \sum_{i \neq j} \Delta_i^* \Delta_j \left(k_i k_j - \frac{Q_i Q_j}{4}\right) + \sum_{i \neq j} \Delta_i^* \Delta_j \frac{1}{2} (k_j Q_i - k_i Q_j) = \\ & = |\Delta_0^s|^2 \left(|\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4}\right) + \frac{1}{2} \sum_{i \neq j} \Delta_i^* \Delta_j |\mathbf{k}| |\mathbf{Q}| \sin(\theta) (-1)^j = \end{aligned}$$

<sup>5</sup>We defined:  $Q_\mu \equiv (0, \mathbf{Q})$

$$\begin{aligned}
&= |\Delta_0^s|^2 \left( |\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4} \right) + \frac{1}{2} |\mathbf{k}| |\mathbf{Q}| (\Delta_1^* \Delta_2 \sin(\theta) + \Delta_2^* \Delta_1 \sin(-\theta)) = \\
&= |\Delta_0^s|^2 \left( |\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4} \right) + \frac{1}{2} |\mathbf{k}| |\mathbf{Q}| \sin(\theta) (\Delta_1^* \Delta_2 - \Delta_2^* \Delta_1)
\end{aligned}$$

Having introduced  $\theta$  defined as the angle between  $\mathbf{Q}$  and  $\mathbf{k}$ . Arbitrarily choosing the direction of  $\mathbf{Q}$  this angle can also be regarded as the variable  $\theta$  over which one integrates after the sums are converted to integrals, and the integrals are, in turn, converted in polar coordinates. One can now write the dispersion relation in implicit form:

$$\begin{aligned}
0 = & \left( -\omega^2 + |\mathbf{k}|^2 + m_s^2 + \frac{|\mathbf{Q}|^2}{4} \right)^2 - |\mathbf{k}|^2 |\mathbf{Q}|^2 \cos^2(\theta) - 4 |\Delta_0^s|^2 \left( |\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4} \right) + \\
& - 2 \sin(\theta) |\mathbf{k}| |\mathbf{Q}| (\Delta_1^* \Delta_2 - \Delta_2^* \Delta_1)
\end{aligned}$$

which then yields:

$$\begin{cases} E'_\pm(\mathbf{k}) = \sqrt{m_s^2 + |\mathbf{k}|^2 + \frac{|\mathbf{Q}|^2}{4}} \pm J \\ J = \sqrt{4 |\Delta_0^s|^2 \left( |\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4} \right) + |\mathbf{k}|^2 |\mathbf{Q}|^2 \cos^2(\theta) + 2 \sin(\theta) |\mathbf{k}| |\mathbf{Q}| (\Delta_1 \Delta_2^* - \Delta_2 \Delta_1^*)} \end{cases}$$

As expected the relation just found coincides with the unperturbed case when setting  $\mathbf{Q} = 0$  and we also note that, writing down the Taylor-series expansion for  $E'_\pm(\mathbf{k})$  using  $|\mathbf{Q}|$  as the expansion parameter one can formally write the result of this section as:

$$E'_\pm(\mathbf{k}) = E_\pm(\mathbf{k}) + |\mathbf{Q}| f_\pm(\mathbf{k}) + \frac{|\mathbf{Q}|^2}{2} g_\pm(\mathbf{k}) + O(|\mathbf{Q}|^3)$$

for an opportune choice of the functions  $f_\pm$  and  $g_\pm$ ; grouping in one single term all the corrections due to the twist to the original dispersion relations, at all orders, we obtain a formal expression which will be frequently used in what follows:

$$E'_{\pm} = E_{\pm} + \Delta E_{\pm} \quad (7.6)$$

### 7.1.2 Free energy and $\rho_0$

Now we need to re-derive the partition function for the system, to evaluate how it is changed by the infinitesimal twist to the order parameter. The partition function for the unperturbed system, keeping into account the spin multiplicity, is to be written as:

$$Z = Z_0^{(2s+1)} \quad Z_0 = \sum_{\mathbf{k}} e^{-\beta(E_+(\mathbf{k})+E_-(\mathbf{k}))}$$

where  $s$  denotes the spin. On the other hand, after having imposed the twist, the new partition function can be symbolically written as follows:

$$Z' = Z_0'^{(2s+1)} \quad Z_0' = \sum_{\mathbf{k}} e^{-\beta(E_+(\mathbf{k})+E_-(\mathbf{k})+\Delta E_++\Delta E_-)}$$

One can put in evidence the infinitesimal contribution, and then write the Taylor series expansion to the first order in  $\Delta E_{\pm}$ :

$$\begin{aligned} Z_0' &= \sum_{\mathbf{k}} e^{-\beta(E_+(\mathbf{k})+E_-(\mathbf{k}))} \cdot e^{-\beta(\Delta E_++\Delta E_-)} = \\ &= \sum_{\mathbf{k}} e^{-\beta(E_+(\mathbf{k})+E_-(\mathbf{k}))} \cdot (1 - \beta(\Delta E_+ + \Delta E_-)) = Z_0 + Z_0 \langle -\beta(\Delta E_+ + \Delta E_-) \rangle \end{aligned}$$

where  $\langle \# \rangle$  denotes the ensemble average. Remembering that  $\rho_s \propto \Delta F$  we are interested in calculating the free energy variation:

$$\begin{aligned} \Delta F &= -\frac{1}{\beta} (\ln(Z') - \ln(Z)) = -\frac{(2s+1)}{\beta} \ln \left( \frac{Z_0 + Z_0 \langle -\beta(\Delta E_+ + \Delta E_-) \rangle}{Z_0} \right) = \\ &= -\frac{2}{\beta} \ln(1 + \langle -\beta(\Delta E_+ + \Delta E_-) \rangle) \approx -\frac{2}{\beta} \langle -\beta(\Delta E_+ + \Delta E_-) \rangle = 2 \langle \Delta E_+ + \Delta E_- \rangle \end{aligned}$$

$$\implies \boxed{\Delta F = 2\langle \Delta E_+ + \Delta E_- \rangle}$$

The complete expression for the superfluid density, as seen in eq. 2.13, is:

$$\Delta F = F(\mathbf{Q}) - F(\mathbf{Q} = 0) = \frac{1}{2}\rho m v_s^2$$

and by noting that  $\mathbf{v}_s = \frac{\mathbf{Q}}{2m} \Rightarrow |\mathbf{v}_s|^2 = \frac{|\mathbf{Q}|^2}{4m^2}$ , it follows that:

$$\Delta F = \frac{1}{2}\rho_s m \frac{|\mathbf{Q}|^2}{4m^2} = \rho_s \frac{|\mathbf{Q}|^2}{8m}$$

Solving for  $\rho_s$  the final expression for the superfluid density is readily obtained as:

$$\rho_{s,0} = \frac{8m}{|\mathbf{Q}|^2} \Delta F = \frac{16m}{|\mathbf{Q}|^2} \langle \Delta E_+ + \Delta E_- \rangle$$

and can be evaluated as soon as one is able to calculate  $\langle \Delta E_+ + \Delta E_- \rangle$ ; in order to accomplish this goal one needs to solve a couple of issues, which remained hidden so far and will be discussed in detail in the following section.

### 7.1.3 Calculation of $\langle \Delta E_+ + \Delta E_- \rangle$

The two issues briefly mentioned in the previous subsection are the following ones:

- The two quantities  $\Delta E_+$  and  $\Delta E_-$ , as defined in eq. 7.6, are divergent for small momenta when taken singularly. Their sum, however, does converge as one may expect. So  $\Delta E_+ + \Delta E_-$  of which we want to calculate the ensemble average is not to be calculated naively as the sum of the two contributions, from the two branches of the spinon dispersion relation, but it is better calculated after some algebraic manipulation.

- As previously noted, when imposing the twist on the  $2 \times 2$  matrix  $\Gamma$  we changed the dynamics of the spinons inducing a shift in the speed of all spinons. This effect has yet to be more thoroughly analyzed, and, eventually, to be kept into account; that is the case, as already briefly mentioned, when working on a lattice using an UV cutoff.

To solve the first issue one can conveniently think of  $\Delta E_+ + \Delta E_-$  as  $\Delta(E_+ + E_-)$ , doing the calculation in the following way:

$$\left\{ \begin{aligned} E'_\Sigma &= E'_+ + E'_- = \sqrt{E_+^2 + E_-^2 + 2E_+E_-} = \\ &= \sqrt{2 \cdot \left(m_s^2 + |\mathbf{k}|^2 + \frac{|\mathbf{Q}|^2}{2}\right) + 2\sqrt{\left(m_s^2 + |\mathbf{k}|^2 + \frac{|\mathbf{Q}|^2}{2}\right)^2 - J^2}} \\ J^2 &= 4|\Delta_0^s|^2 \left(|\mathbf{k}|^2 - \frac{|\mathbf{Q}|^2}{4}\right) + |\mathbf{k}|^2 |\mathbf{Q}|^2 \cos^2(\theta) + 2 \sin(\theta) |\mathbf{k}| |\mathbf{Q}| (\Delta_1 \Delta_2^* - \Delta_2 \Delta_1^*) \end{aligned} \right.$$

having defined  $E_\Sigma \equiv E_+ + E_-$  and consistently using the prime for the “twisted” versions of original quantities. It follows that:

$$E'_\Sigma = (E_+ + E_-) + \underbrace{|\mathbf{Q}| \frac{\partial E'_\Sigma}{\partial |\mathbf{Q}|} \Big|_{|\mathbf{Q}|=0}}_{E_1} + \underbrace{\frac{|\mathbf{Q}|^2}{2!} \frac{\partial^2 E'_\Sigma}{\partial |\mathbf{Q}|^2} \Big|_{|\mathbf{Q}|=0}}_{E_2} + O(|\mathbf{Q}|^3)$$

$\Delta E_\Sigma \equiv \Delta E_+ + \Delta E_-$

and the expansion is no longer divergent at any order. It is now easily argued that  $E_1$  is going to contain only terms  $\propto \sin(\theta)$  which are not going to give any contribution once we calculate the ensemble average:

$$E_1 = |\mathbf{Q}| \frac{\partial E'_\Sigma}{\partial |\mathbf{Q}|} \Big|_{|\mathbf{Q}|=0} = |\mathbf{Q}| |\mathbf{k}| \frac{\sin(\theta) (\Delta_1^* \Delta_2 - \Delta_1 \Delta_2^*)}{(E_+ + E_-)(E_+ \cdot E_-)} \implies \langle E_1 \rangle = 0$$

The calculation for the second order term  $E_2$  is very lengthy and has been carried out with Wolfram Mathematica<sup>®</sup>:

$$\begin{cases} E_2 = \frac{|\mathbf{Q}|^2}{2!} \left. \frac{\partial^2 E'_\Sigma}{\partial |\mathbf{Q}|^2} \right|_{|\mathbf{Q}|=0} = \frac{|\mathbf{Q}|^2}{2} (E_+ + E_-) \left[ \frac{\frac{1}{2} - A + B}{(E_+ + E_-)^2} - \frac{|\mathbf{k}|^2 \sin^2(\theta) (\Delta_1 \Delta_2^* - \Delta_1^* \Delta_2)^2}{(E_+ + E_-)^2 (E_+ \cdot E_-)^2} \right] \\ A = \frac{|\mathbf{k}|^2 \sin^2(\theta) (\Delta_1 \Delta_2^* - \Delta_1^* \Delta_2)^2}{(E_+ \cdot E_-)^3} \\ B = \frac{m_s^2 + 2|\Delta|^2}{2(E_+ \cdot E_-)} \end{cases}$$

The ensemble average for the above expression for  $E_2$  will be calculated numerically and will then be used for plotting  $\rho_{s,0}$ , as  $\rho_{s,0} \propto \langle \Delta E_+ + \Delta E_- \rangle = \langle \Delta E_\Sigma \rangle = \langle E_2 \rangle$ .

The second issue mentioned above arises because of the transformation in eq. 7.5 does not let the physics of the system untouched. In order to understand how the physics are changed it is useful to visualize the area of the momentum space in which one sums when evaluating the partition function  $Z$ : how does  $Z$  change when adding a constant offset to all speed of all particles? In absence of any UV cutoff it is clear that:

$$\sum_{\mathbf{k}, \mathbf{k} \in \mathbb{R}^2} = \sum_{\mathbf{k} + \mathbf{Q}, \mathbf{k} \in \mathbb{R}^2}$$

for any constant two-dimensional vector  $\mathbf{k}$ . On the other hand one cannot say the same when using an UV cutoff, because:

$$\sum_{\mathbf{k}, \mathbf{k} \in \mathbb{R}^2, |\mathbf{k}| \leq \Lambda} \neq \sum_{\mathbf{k} + \mathbf{Q}, \mathbf{k} \in \mathbb{R}^2, |\mathbf{k}| \leq \Lambda}$$

as in the l.h.s. the sum is calculated over the area of a circle of radius  $\Lambda$  centered on the origin, while in the r.h.s. the sum runs over an identical circle, but centered in  $-\mathbf{Q}$ ; going more into detail the effects are easily seen to be of order  $|\mathbf{Q}|^2$  when  $|\mathbf{Q}| \ll 1$  and cannot then be neglected as far as the current calculation is concerned.

This issue is solved by removing “by hand” from the free energy a contribution which will take into account the extra speed acquired by the spinons. By calling  $\Delta F^{\text{twist}+\text{boost}}$  the quantity already calculated it is clear that we

need to subtract from this quantity a term which account for the shift of the integration domain in momentum space, we will refer to this term as  $\Delta F^{\text{boost}}$ , so that, in formulas:

$$\rho_s \propto \Delta F^{\text{twist}} = \Delta F^{\text{twist+boost}} - \Delta F^{\text{boost}}$$

The whole calculation for  $\Delta F^{\text{boost}}$  will not be reported here, as it follows the very same steps used in calculating  $E_1$  and  $E_2$ ; briefly one needs to evaluate differences in the dispersion relation when the speed of the spinons is shifted as  $\mathbf{k} \rightarrow \mathbf{k} + \frac{\mathbf{Q}}{2}$ ; this is easily done by Taylor-expanding as follows:

$$E_{\pm} \left( \mathbf{k} + \frac{\mathbf{Q}}{2} \right) = E_{\pm}(\mathbf{k}) + |\mathbf{Q}| l_{\pm}(\mathbf{k}) + \frac{|\mathbf{Q}|^2}{2!} m_{\pm}(\mathbf{k}) + \dots$$

for an adequate choice of the  $l_{\pm}$  and  $m_{\pm}$  functions; consistently with the previous case when taking the ensemble average there is no contribution at the first order.

#### 7.1.4 Final results for $\rho_{s,0}$

The contribution to the superfluid density from  $S_{\text{eff}}^{s,0}$  can then be calculated numerically using the procedure explained in the previous subsection, the final result can be observed in fig. 7.1; as already explained the most important feature of this contribution is that it goes to zero only when  $T \geq T_{ps}$ , so that there is a non-negligible superfluid density even in the  $T_c \leq T \leq T_{ps}$  interval.



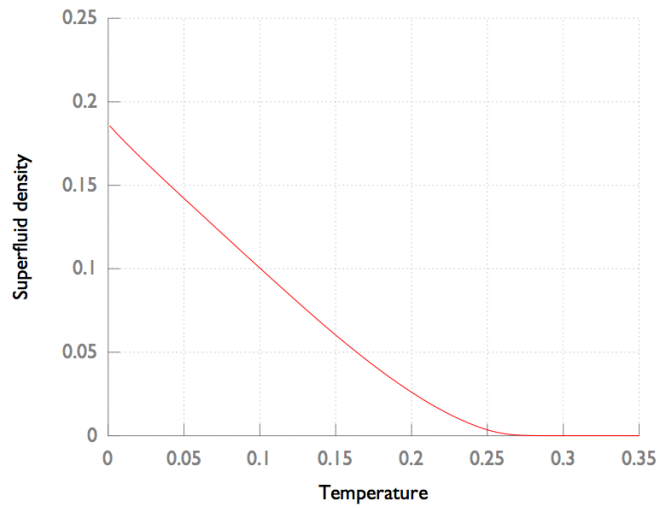


Figure 7.1: The contribution to (mechanically-defined) superfluid density coming from  $S_{\text{eff}}^{s,0}$ . Both in the  $x$  and the  $y$  axis arbitrary units are used, the doping has been set to  $\delta = 0.14$ , as a consequence  $T_{ps} \approx 0.27$ .

## 7.2 Calculation of $\rho_{s,2}$

For the calculation of the gauge fluctuations contribution to superfluid density, which will turn out to play an essential role like they do for pairing, our starting point will be the partition function for the gauge contribution to the model, as defined in section 6.3; however in section 6.3 we were interested in calculating the partition function only in order to derive the gap equation, so that the phase  $\phi^s$  could be self-consistently neglected, as also discussed in [7] and in [36]. On the other hand we now want to calculate the partition function to obtain the free energy and ultimately the superfluid density, so that we are no longer allowed to neglect the phase: the partition function has then to be written as derived in eq. 6.10, using the gauge invariant fields  $a_\mu$  and  $\phi$ , as:

$$Z_g = \int \mathcal{D}a_\mu \mathcal{D}\phi e^{-\int d^3x \mathcal{L}_g[a_\mu, \phi]} \quad (7.7)$$

$$\mathcal{L}_g = \frac{1}{6\pi M} \left\{ [\partial_\mu a_\nu - \partial_\nu a_\mu]^2 + |\Delta_0^s|^2 \eta^{\mu\nu} \left( a_\mu - \frac{1}{2} \partial_\mu \phi \right) \left( a_\nu - \frac{1}{2} \partial_\nu \phi \right) \right\} \quad (7.8)$$

where  $\mathcal{L}_g$  is the (Euclidean) Lagrangian for the system, and  $\eta^{\mu\nu}$  denotes the anisotropic metric tensor,  $\eta^{\mu\nu} \equiv \text{diag}(2, 1, 1)$ .

We note that the model described by the partition function and the Lagrangian in equations 7.7 and 7.8 are quite similar to the model derived in section 6.3 in which we neglected the phase. More specifically we still find a three-dimensional anisotropic gauged XY model, the only difference being that the relevant variable is now  $\phi$ , instead of  $\phi^h$ ; moreover, as we will shortly see, an effective theory can be derived with a 3D XY model with  $\phi^s$  as the angular variable.

As noted in [7] when writing down the partition function starting from the Lagrangian above one must be careful to separate physical and non-physical

degrees of freedom; namely one must take into account that, although  $a_\mu$  and  $\phi$  are gauge invariant objects, nonetheless the  $U(1)$   $h/s$  gauge symmetry has not been fixed yet, so that the naive path integral  $Z = \int \mathcal{D}a_\mu \mathcal{D}\phi e^{-S[a_\mu, \phi]}$  will integrate over gauge-equivalent configurations and, ultimately, diverge. Referring again to [7] and citations therein, particularly [37], the right procedure to derive the partition function consists in reinstating the original non-gauge invariant fields, i.e. the phases  $\phi^h$ ,  $\phi^s$  and the  $A_\mu$  field, by means of the relations:

$$\begin{cases} a_\mu \equiv A_\mu - \frac{1}{2} \partial_\mu \phi^h \\ \phi = \phi^h - \phi^s \end{cases}$$

obtaining the following Lagrangian

$$\begin{aligned} \mathcal{L}_g = \frac{1}{6\pi M} & \left\{ [\partial_\mu A_\nu - \partial_\nu A_\mu]^2 - 2\partial_\mu A_\nu [\partial^\mu, \partial^\nu] \phi^h + \right. \\ & \left. + \frac{1}{4} ([\partial_\mu, \partial_\nu] \phi^h)^2 + |\Delta_0^s|^2 \eta^{\mu\nu} \left( A_\mu - \frac{1}{2} \partial_\mu \phi^s \right) \left( A_\nu - \frac{1}{2} \partial_\nu \phi^s \right) \right\} \end{aligned} \quad (7.9)$$

We now note that the term  $2\partial_\mu A_\nu [\partial^\mu, \partial^\nu] \phi^h$  can be neglected in a low-energy approximation being of order three in the derivatives, while the other terms appearing in  $\mathcal{L}_g$  are of order two at most. As a side effect of this approximation the dynamics of the holon phase is now completely decoupled from the other fields, while the spinon phase and the  $A_\mu$  gauge field are coupled by only one term which can be eliminated by an adequate choice of the gauge fixing. We can now write the Lagrangian as:

$$\begin{aligned} \mathcal{L}_g = \frac{1}{6\pi M} & \left\{ [\partial_\mu A_\nu - \partial_\nu A_\mu]^2 + \frac{1}{4} ([\partial_\mu, \partial_\nu] \phi^h)^2 \right. \\ & \left. + |\Delta_0^s|^2 \eta^{\mu\nu} \left( A_\mu - \frac{1}{2} \partial_\mu \phi^s \right) \left( A_\nu - \frac{1}{2} \partial_\nu \phi^s \right) \right\} \end{aligned} \quad (7.10)$$

which can in turn be rewritten in the following way:

$$\mathcal{L}_g = A_\mu K^{\mu\nu} A_\nu + \frac{|\Delta_0^s|}{24\pi M} \eta^{\mu\nu} \partial_\mu \phi^s \partial_\nu \phi^s - \frac{|\Delta_0^s|^2}{6\pi M} \eta^{\mu\nu} A_\mu \partial_\nu \phi^s + H(\phi^h) \quad (7.11)$$

$$K_{\mu\nu} = \frac{1}{3\pi M} \left[ \partial^\mu \partial^\nu - \partial^2 g^{\mu\nu} + \frac{|\Delta_0^s|^2}{2} \eta^{\mu\nu} \right] = \frac{1}{3\pi M} [\partial^\mu \partial^\nu - \partial^2 g^{\mu\nu} + m^{\mu\nu}] \quad (7.12)$$

emphasizing the fact that the gauge field  $A_\mu$  describes a theory which is akin to that of a massive boson, while on the other hand we find that the dynamics of the spinon phase are those of a three dimensional anisotropic XY model. The XY model can be deemed as ungauged, as opposed to the model we started from at beginning of the present section, as long as it is understood that the term  $\sim \eta^{\mu\nu} A_\mu \partial_\nu \phi^s$  will be treated separately, i.e. eliminated by an appropriate gauge choice. The dynamics of the holon phase are included in  $H(\phi^h)$  and will be integrated out because, as it will be clear shortly, they do not play any specific role in how we decided to evaluate  $\rho_s$ . Also in eq. 7.12 the tensor  $m^{\mu\nu}$  has been straightforwardly defined; here we note that it can be seen as a “pseudo-mass” tensor and that if it were diagonal it would be a fully fledged mass for the  $A_\mu$  gauge field.

In order to give a complete treatment we should now include the holon contribution to the partition function, this aim could be achieved as seen in section 6.3 by redefining the matrix  $m^{\mu\nu}$  as follows:

$$\begin{pmatrix} |\Delta_0^s|^2 & 0 & 0 \\ 0 & \frac{1}{2} |\Delta_0^s|^2 & 0 \\ 0 & 0 & \frac{1}{2} |\Delta_0^s|^2 \end{pmatrix} \longrightarrow \begin{pmatrix} |\Delta_0^s|^2 + \tilde{c}_2 & 0 & 0 \\ 0 & \frac{1}{2} |\Delta_0^s|^2 + f(\mathbf{k}) & 0 \\ 0 & 0 & \frac{1}{2} |\Delta_0^s|^2 + f(\mathbf{k}) \end{pmatrix} \quad (7.13)$$

with  $\tilde{c}_2 = 3\pi M c_2$  and  $f(\mathbf{k}) = 3\pi M c_1 \sqrt{v_F^2 k_+^2 + v_\Delta^2 k_-^2}$ . However it can be shown that this contribution is subleading with respect to the other terms appearing in the Lagrangian and can be consistently neglected as far as the current treatment is concerned. In order to show that we need to exploit three facts:

- Firstly we need to recall that  $M$  is defined as  $M \equiv \sqrt{m_s^2 - 2|\Delta_0^s|^2}$ .

- Secondly, we also recall that, as thoroughly discussed in the introductory section of this chapter,  $\rho_{s,2}$  can only be non-zero below the critical temperature and that  $|\Delta_0^s|^2$  is a monotonically decreasing function of temperature.
- Lastly, we anticipate that, as it will be shown in subsection 7.2.2, for  $T \sim T_c$  one sees that  $|\Delta_0^s|_c^2 \approx \frac{m_s^2}{2} + O\left(\frac{m_s^4}{576\pi^2 T_c^2}\right)$ .

Hence it is now straightforward to exclude the holon contributions by noting that the Lagrangian terms coming from the holon contribution all have a prefactor  $3\pi M$  with respect to the other terms, which in the range  $0 < T \leq T_c$  roughly evaluates to:

$$3\pi M = 3\pi \sqrt{m^2 - 2|\Delta_0^s|^2} \approx 3\pi \sqrt{m_s^2 - m_s^2 + O\left(\frac{m_s^4}{576\pi^2 T_c^2}\right)} \approx O\left(\frac{m_s^2}{8T_c}\right)$$

which is numerically small and, for typical values of  $m_s$  and  $T_c$  will be at least two orders of magnitude smaller than the other terms.

Referring to the theory described by eq. 7.11 and 7.12 where the gauge-invariance is left explicit, we now note that it can be fixed by using the Faddeev-Popov procedure by integrating only over the configurations which satisfy a functional constraint expressed choosing a gauge fixing function  $F$ :

$$Z_g = \mathcal{N} \int \mathcal{D}A_\mu \mathcal{D}\phi^s \left| \frac{\delta F}{\delta \Lambda} \right| e^{-\int d^3x \mathcal{L}_g} \quad (7.14)$$

The gauge fixing function will be chosen conveniently at a later time, it is implied that starting from eq. 7.14 the Lagrangian does not contain the  $\phi^h$  field any longer, as it has been integrated out and its contribution is included in the multiplicative constant  $\mathcal{N}$ ; nonetheless we will continue to refer to this new Lagrangian as  $\mathcal{L}_g$ . As our final aim is to evaluate the differences in the action (and ultimately in the free energy) when a twist  $\Delta^c \rightarrow \Delta^c e^{i\vec{Q}\cdot\vec{x}}$  is applied to the superconductivity order parameter, we put into practice the twist as

$$\phi^s \longrightarrow \phi^s - Q_\mu x^\mu \quad (7.15)$$

having defined  $Q_\mu \equiv (0, \vec{Q})$ . It is to be noted that, in a completely equivalent way, one could have expressed the theory in terms of  $\phi^h$  implementing the twist as  $\phi^h \longrightarrow \phi^h + Q_\mu x^\mu$ , the gauge invariance ensuring that the procedure must not have any effect on the superfluid density, which is a physical observable; in that case, however, one could not have integrated out the  $\phi^h$  variable as done in the present treatment. After the twist just discussed the theory described by eq. 7.14 changes as follows:

$$\mathcal{L}_g \longrightarrow \mathcal{L}_g + \Delta\mathcal{L}_g$$

$$\Delta\mathcal{L}_g = \frac{|\Delta_0^s|^2}{6\pi M} \left( -\eta^{\mu\nu} A_\mu Q_\nu + \frac{1}{2}\eta^{\mu\nu} Q_\mu \partial_\nu \phi^s + \frac{1}{4}\eta^{\mu\nu} Q_\mu Q_\nu \right) \quad (7.16)$$

It is easily seen in eq. 7.16 that the net effects of the twist are, in the approximation just described:

$$\begin{aligned} \Delta\mathcal{L}_{\text{gauge}} &= -\frac{|\Delta_0^s|^2}{6\pi M} \eta^{\mu\nu} Q_\nu A_\mu = J^\mu A_\mu \\ \Delta\mathcal{L}_{\text{XY}} &= \frac{1}{24\pi M} \left( |\Delta_0^s|^2 \eta^{\mu\nu} Q_\mu Q_\nu + 2|\Delta_0^s|^2 \eta^{\mu\nu} Q_\mu \partial_\nu \phi^s \right) \end{aligned}$$

i.e. a current  $J_\mu A^\mu$  coupled to the  $A_\mu$  field and the contribution to the superfluid density of a anisotropic XY model, where the imaginary time has been promoted to the role of a fully-fledged spatial dimension and the “coupling constant”  $\frac{|\Delta_0^s|^2}{24\pi M}$  plays the role of the inverse temperature. One can convince themselves of this fact by writing down the Lagrangian for an anisotropic three-dimensional XY model (from now on A3DXY), which in its continuum version reads<sup>6</sup>:

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<sup>6</sup>The A3DXY model will be analyzed more thoroughly in subsection 7.2.2

$$\mathcal{L} = J\eta^{\mu\nu}\partial_\mu\phi^s\partial_\nu\phi^s$$

and by observing that  $\Delta\mathcal{L}_{\text{xy}}$  is actually (up to a global multiplicative constant) how the action varies upon the twist in eq. 7.15, or equivalently by noting that  $\Delta\mathcal{L}_{\text{XY}}$  corresponds to whole variation when the  $A_\mu$  field is set to zero. We postpone the discussion of this term to section 7.2.2, noting that it has been thoroughly analyzed in scientific literature (e.g. [38] and [39]), and that while there is no known closed-form expression for the superfluid density of that model, it is quite easily calculated with Montecarlo techniques.

We now focus on the other contributions, wanting to show that they are null or negligible, so that as far as the superfluid density is concerned the superfluid density will turn out to be essentially XY-like. As already noted  $\Delta\mathcal{L}_{\text{gauge}}$  can be thought of as a contribution given by a  $J_\mu = (6\pi M)^{-1}|\Delta_0^s|^2 Q_\mu$  current coupled to the  $A_\mu$  gauge field. Briefly switching to the hamiltonian formalism we can note that this term gives a negative contribution to the free energy by means of Bogoliubov inequality:

$$\mathcal{H} = \mathcal{H}_0 + J_\mu A^\mu \implies F \leq F_0 + J_\mu \langle A^\mu \rangle_0 = F_0$$

denoting with  $\mathcal{H}_0$  the hamiltonian for the system in the standard case, and with  $F_0$  and  $F$  the free energy calculated, respectively, from  $\mathcal{H}_0$  and from  $\mathcal{H}$ ;  $\langle \# \rangle_0$  is the ensemble average defined by  $\mathcal{H}_0$ .

Moreover, by readapting the calculations in [40], particularly the convexity lemma used in the demonstration for Bogoliubov inequality, formally exchanging the roles played by  $\lambda$  and each component of  $\mathbf{Q}$  one can demonstrate that:

$$\rho_s \propto \frac{d^2 F}{dQ_i^2} \leq 0$$

for  $i = 1, 2$  so that the contribution to superfluid density arising from  $J_\mu A^\mu$  is also negative. We search then for a lower bound to keep this term

close to zero; in order to do so it is convenient to go back to the path-integral formalism as in eq. 7.14; we can now conveniently choose the gauge-fixing function  $F$  so that the  $A_\mu$  and  $\phi^s$  fields are decoupled and the A3DXY model is almost completely retained in the procedure:

$$F = \alpha \cdot m^{\mu\nu} (\partial_\mu A_\nu) \phi^s - \frac{1}{2\alpha} \phi^s - \omega(x) \quad (7.17)$$

for an arbitrary real constant  $\alpha$ . With this gauge fixing choice, after having completed the Faddeev-Popov procedure the partition function reads:

$$\begin{cases} Z = \int \mathcal{D}A_\mu \mathcal{D}\phi^s e^{-S[A_\mu] - S[\phi^s]} \\ S[A_\mu] = \frac{1}{3\pi M} \int d^3x A_\mu \left( -\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu + m^{\mu\nu} - \alpha^2 m^{\mu\mu'} m^{\nu\nu'} \partial_{\mu'} \partial_{\nu'} \right) A_\nu \\ S[\phi^s] = \frac{1}{12\pi M} \int d^3x \phi^s \left( -\frac{|\Delta_0^s|^2}{2} \eta^{\mu\nu} \partial_\mu \partial_\nu + \frac{1}{2\alpha^2} \right) \phi^s \end{cases}$$

We note that as a result of the Faddeev-Popov procedure two new terms are introduced in the action, a gauge breaking term in the  $A_\mu$  sector and a spurious mass term in the phase sector. In order to eliminate the mass term for the phase field, which is clearly an artifact of the gauge fixing, one must take the limit  $\alpha \rightarrow \infty$ : this choice is commonly referred to as the Landau gauge; however in scientific literature it is more customary to use a gauge parameter  $\xi \propto \frac{1}{\alpha}$ , so that the Landau gauge is defined by  $\xi = 0$ . It is also worth emphasizing that the Landau gauge is the only allowed gauge choice, because, in case  $\phi^s$  should not be a gaussian variable, a term  $\sim m\phi_s^2$  would not even be defined. The gauge choice does not affect the  $A_\mu$  sector, as we will demonstrate shortly that  $\alpha^2 m^{\mu\mu'} m^{\nu\nu'} \partial_{\mu'} \partial_{\nu'}$  gives a negligible contribution, and effectively eliminates the mass term; the action  $S[\phi^s]$  is now, up to 4-divergences in the integrand, the one of an anisotropic three-dimensional XY model.

As the two fields  $A_\mu$  and  $\phi^s$  are now decoupled, so that  $Z = Z_{A_\mu} Z_{\phi^s}$ , it is also clear that they are going to contribute separately to free energy, as



$F = F_{A_\mu} + F_{\phi^s}$ ; we now focus on  $F_{A_\mu}$ . We can formally carry out the gaussian integral, integrating away the current, recalling that we are not interested in an analytical closed form for  $Z_{A_\mu}$ , as we would rather study how the additional term  $\Delta\mathcal{L}_{\text{gauge}}$  in the Lagrangian modifies  $Z_{A_\mu}$  with respect to  $Z_0 \equiv Z_{A_\mu}|_{\Delta\mathcal{L}_{\text{gauge}}=0}$ . The partition function is then given by:

$$Z_{A_\mu} = \int \mathcal{D}A_\mu \exp \left[ \int d^3x \left( -\frac{1}{2} A_\mu L^{\mu\nu} A_\nu - J_\mu A^\mu \right) \right]$$

having defined:

$$L^{\mu\nu} = \frac{2}{3\pi M} \left( -\partial^2 g^{\mu\nu} + \partial^\mu \partial^\nu + m^{\mu\nu} - \alpha^2 m^{\mu\mu'} m^{\nu\nu'} \partial_{\mu'} \partial_{\nu'} \right)$$

and the gaussian integral yields as a result:

$$Z_{A_\mu} = Z_0 \exp \left[ \int d^3x d^3y J_\mu(x) (L^{-1})^{\mu\nu}(x-y) J_\nu(y) \right]$$

Due to the system being isotropic as far as the *spatial* directions are concerned, it is easily seen that the superfluid density cannot depend on the direction of  $\mathbf{Q}$ : we are then free to choose  $J_\mu = \left( 0, (6\pi M)^{-1} |\Delta_0^s|^2 |\mathbf{Q}|, 0 \right)$ ; this is fully equivalent to adopting a frame of reference where the current  $J_\mu$  has the aforementioned form, and that frame of reference can always be reached by spatial rotations. It follows that:

$$\begin{aligned} \frac{Z_{A_\mu}}{Z_0} &= \exp \int d^3x d^3y J_1(x) (L^{-1})^{11}(x-y) J_1(y) = \\ &= \exp \left[ \frac{|\Delta_0^s|^4}{(6\pi M)^2} |\mathbf{Q}|^2 \int d^3x d^3y (L^{-1})^{11}(x-y) \right] \end{aligned} \quad (7.18)$$

In order to demonstrate that the gauge field contribution is indeed negligible we must show that  $\Delta F = -\beta^{-1} \ln \left( \frac{Z_{A_\mu}}{Z_0} \right) \sim 0$ , the contribution from the  $J_\mu$  current to the superfluid density being proportional to  $\Delta F$ . To be able to do so one must note that in eq. 7.18 only the (1, 1) component of the  $L^{\mu\nu}$  matrix appears, so that we can switch to momentum space representation where the  $L^{\mu\nu}$  has the following form:

$$L^{\mu\nu} = \frac{2}{3\pi M} \left( p^2 g^{\mu\nu} - p^\mu p^\nu + m^{\mu\nu} + \alpha^2 m^{\mu\mu'} m^{\nu\nu'} p_{\mu'} p_{\nu'} \right)$$

and then calculate the component we need as  $(L^{-1})^{1,1} = \frac{1}{\det(L)} \begin{vmatrix} L^{0,0} & L^{0,2} \\ L^{2,0} & L^{2,2} \end{vmatrix}$ .

The calculation is quite lengthy and cumbersome and has been carried out with the aid of Wolfram Mathematica<sup>®</sup>; before analyzing the results of this calculation is worth discussing the analogous result in a simpler similar theory, i.e. a massive vector boson with mass  $\mu$ . Such a theory, in its gauge-fixed version, leaving the gauge parameter  $\xi$  explicit, is described by a Lagrangian of the form  $\mathcal{L} \sim A_\mu C^{\mu\nu} A_\nu$  with

$$C^{\mu\nu} = k^2 g^{\mu\nu} - \left( 1 - \frac{1}{\xi} \right) k^\mu k^\nu + \mu^2 g^{\mu\nu}$$

and the associated propagator in momentum space for the  $A_\mu$  field is (see for instance [41]):

$$(C^{-1})^{\mu\nu} = \frac{1}{k^2 + \mu^2} \left( g^{\mu\nu} - (1 - \xi) \frac{k^\mu k^\nu}{k^2 + \xi\mu^2} \right) \quad (7.19)$$

It is worth noting that when calculating an integral such the one in eq. 7.18 the expression in eq. 7.19 can be simplified, neglecting the term  $(1 - \xi) \frac{k^\mu k^\nu}{k^2 + \xi\mu^2}$ , as it will work on conserved currents for which the condition  $k_\mu J^\mu = 0$  holds. Going back to the case relevant for the present thesis, the aforementioned computer calculation for  $(L^{-1})^{1,1}$  yields<sup>7</sup>:

$$(L^{-1})^{1,1} = \frac{\mu^2 + p_1^2 + p_2^2}{(\mu^2 + p^2)(\mu^2 + p_1^2)} + \frac{p_1^2 p_2^2}{\mu^2 (2\mu^2 + 2p^2)(\mu^2 + p_1^2)} - \frac{\alpha^2 p_2^2}{\mu^2 (\mu^2 + 2\alpha^2 p^2)}$$

having defined<sup>8</sup>  $\mu \equiv \frac{|\Delta_0^s|^2}{2}$ . As already discussed the only suitable gauge choice is the Landau gauge, i.e.  $\alpha \rightarrow \infty$ ; when taking this limit  $(L^{-1})^{1,1}$

<sup>7</sup>A global  $\frac{3\pi M}{2}$  factor has been omitted for clarity's sake, in will be reinstated when needed.

<sup>8</sup>So that we can rewrite the pseudo-mass matrix as:  $m^{\mu\nu} = \text{diag}(2\mu, \mu, \mu)$

becomes:

$$\lim_{\alpha \rightarrow \infty} (L^{-1})^{1,1} = \frac{\mu^2 + p_1^2 + p_2^2}{(\mu^2 + p^2)(\mu^2 + p_1^2)} + \frac{p_1^2 p_2^2}{\mu^2 (2\mu^2 + 2p^2)(\mu^2 + p_1^2)} - \frac{p_2^2}{2\mu^2 p^2}$$

Analogously to the previous case we can simplify the expression above by noting that it will work on currents for which the condition  $k_\mu J^\mu = 0$  (no summation) applies; this condition is stronger than being a conserved current, and allows us to neglect the second and the third terms on the right hand side. After some algebraic manipulation we are left with<sup>9</sup>:

$$(L^{-1})^{1,1} = \frac{1}{\mu^2 + p^2} - \frac{p_2^2}{2\mu^2 p^2}$$

We postpone to appendix A the demonstration that the second term in the r.h.s. of the equation above gives no contribution. As a consequence, as far as the present calculation is concerned, our theory is formally equivalent to the one described by  $C^{\mu\nu}$ : in conclusion the integral to calculate is:

$$\frac{Z_{A\mu}}{Z_0} = \exp(W[J]) \quad W[J] = \frac{3\pi M}{2} \int d^3x \int d^3y J_1(x) C^{-1}|_{\xi=1}^{11}(x-y) J_1(y) \quad (7.20)$$

which can be evaluated as follows<sup>10</sup>:

$$\begin{aligned} W[J] &= \frac{3\pi M}{2} \int d^3x \int d^3y J_1(\mathbf{x}) \left[ \int \frac{d^3k}{(2\pi)^3} \frac{e^{ik(x-y)} g^{11}}{k^2 + \mu^2} \right] J_1(\mathbf{y}) = \\ &= \frac{3\pi M}{2} \int dx_0 dy_0 \int d^2x d^2y J_1(\mathbf{x}) \left[ \int \frac{d^3k}{(2\pi)^3} e^{ik_0(x_0-y_0)} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{k^2 + \mu^2} \right] J_1(\mathbf{y}) = \dots \end{aligned}$$

The integration over  $y_0$  gives  $2\pi\delta(k_0)$  which in turn can be used to carry out the integration out  $k_0$ :

<sup>9</sup>The Landau gauge choice is now intended.

<sup>10</sup>Working in (2+1) dimension we use the standard italic notation for a 3-vector, writing spatial-only 2-vectors in bold.

$$\dots = \frac{3\pi M}{2} \int dx^0 \int d^2x d^2y J_1(\mathbf{x}) \left[ \frac{d^2k}{(2\pi)^2} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{|\mathbf{k}|^2 + \mu^2} \right] J_1(\mathbf{y}) = \dots$$

Taking out of the integral sign the currents, which as seen are constant and uniform, rewriting them at the same time into their explicit form, we finally find  $W[J]$  to be:

$$W[J] = \frac{|\Delta_0^s|^4}{24\pi M} \underbrace{\int dx_0}_{=\beta} \int d^2x d^2y V_{\text{Yukawa}}(\mathbf{x} - \mathbf{y}, \mu)$$

with:

$$V_{\text{Yukawa}}(\mathbf{x}, \mu) = \int \frac{d^2k}{(2\pi)^2} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^2 + \mu^2}$$

so that

$$\Delta F = -\beta^{-1} \ln \left( \frac{Z}{Z_0} \right) = -\frac{|\Delta_0^s|^4}{24\pi M} \int d^2x d^2y V_{\text{Yukawa}}(\mathbf{x} - \mathbf{y}, \mu) \quad (7.21)$$

is effectively, up to a multiplicative constant, the electromagnetic self-interaction energy of a charged  $L \times L$  square,  $L$  being the spatial dimension of the system, in a two-dimensional theory of Electromagnetism in which the photon has mass  $\mu \neq 0$ . We now make the following two assumptions, which will be demonstrated in detail respectively in subsection 7.2.1 and in appendix B:

- As already noted  $\Delta F \leq 0$ ; it will be demonstrated that when setting  $\mu = 0$  one actually lowers  $\Delta F$ , so that a lower bound for  $\Delta F' = \Delta F|_{\mu=0}$  will also be a lower bound for  $\Delta F$ .
- When setting  $\mu = 0$  reverts back to standard Electromagnetism in two-dimensions, so that  $\Delta F$  is to be calculated as follows:

$$\Delta F = -L^2 \frac{|\Delta_0^s|^4}{24\pi M} \int_{[0,1]^4} d^2x d^2y V_{\text{Yukawa}}(\mathbf{x} - \mathbf{y}, \mu = 0) = -L^2 \frac{|\Delta_0^s|^4}{24\pi M} I$$

the integral  $I$  just defined will be shown to evaluate to:

$$I = -\frac{-25 + 4\pi + 2 \log(4)}{12} \approx 0,805 \quad (7.22)$$

Now one can refer to the discussion of the contribution of the XY model to superfluid density in subsection 7.2.2 to observe that the contribution to superfluid density arising from the present section is proportional to  $\frac{1}{V} \Delta F \propto |\Delta_0^s|^4$ . For typical values of  $\Delta_s^0$  it is at least two orders of magnitude lower than the other contributions, so that it can be neglected in a very good approximation.

### 7.2.1 Bounds on the non-XY contribution

We asserted without demonstration that when calculating the interaction integral in eq. 7.21, the mass term can be neglected as it only lowers the value of the integral, while we are searching for a suitable lower bound. Our assertion can be written in formulas as an inequality between the Fourier transforms defining two propagators for the  $A_\mu$  gauge field:

$$\int \frac{d^2k}{(2\pi)^2} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^2} \geq \int \frac{d^2k}{(2\pi)^2} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^2 + \mu^2}$$

In order to demonstrate this assertion we will follow the discussion in [42], § 7. Adopting for clarity the notation used therein the assertion above is tantamount to requiring:

$$C(m_1; \mathbf{x} - \mathbf{y}) \leq C(m_2; \mathbf{x} - \mathbf{y}) \text{ when } m_1 \geq m_2 \quad (7.23)$$

where  $C$  is the propagator for the  $A_\mu$  field, defined by:

$$C(m; \mathbf{x}, \mathbf{y}) = C(m; \mathbf{x} - \mathbf{y}) = \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \int e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})} (|\mathbf{p}|^2 + m^2)^{-1} d\mathbf{p} \quad (7.24)$$

where  $d$  is the (spatial) dimensionality of the system. Referring again to [42] one can write down a closed-form expression for the free Euclidean propagator, namely:

$$C(m; \mathbf{x} - \mathbf{y}) = \left(\frac{1}{2\pi}\right)^{-\frac{d}{2}} \left(\frac{m}{|\mathbf{x} - \mathbf{y}|}\right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}}(m|\mathbf{x} - \mathbf{y}|) \quad (7.25)$$

where  $K_i$  is the modified Bessel function of second kind.

This expression is well-behaved in the massless limit, for which one correctly obtains  $C_\gamma \sim -\frac{1}{2\pi} \ln(r)$  for  $d = 2$  so that the inequality we want to prove (in eq. 7.23) can also be proved directly by recalling the properties of the  $K_\nu$  function. However one can also, alternatively, retrace<sup>11</sup> the process of dimensional regularization which leads from eq. 7.24 to eq. 7.25. The propagator for  $A_\mu$  as defined in eq. 7.24 is rewritten in an alternate form by means of the following identity:

$$\frac{1}{p^2 + m^2} = \int_0^\infty \exp[-t(p^2 + m^2)] dt$$

so that:

$$\begin{aligned} C(m; \mathbf{x} - \mathbf{y}) &= \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \int_0^\infty \exp(-tm^2) \int e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})-tp^2} d^d p dt = \\ &= \left(\frac{1}{2\pi}\right)^{\frac{d}{2}} \int_0^\infty \exp\left(-tm^2 - \frac{|\mathbf{x} - \mathbf{y}|^2}{4t}\right) \int \exp(-tq^2) d^d q dt = \\ &= \int_0^\infty t^{-\frac{d}{2}} \exp\left(-tm^2 - \frac{|\mathbf{x} - \mathbf{y}|^2}{4t}\right) dt = \end{aligned}$$

<sup>11</sup>The complete calculations can be found, for instance, in [43].

$$= \left(\frac{1}{2\pi}\right)^{-\frac{d}{2}} \left(\frac{m}{|\mathbf{x}-\mathbf{y}|}\right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}}(m|\mathbf{x}-\mathbf{y}|)$$

By noting that one step before introducing the modified Bessel function of second kind  $K_\nu$  the following inequality holds:

$$\int_0^\infty t^{-\frac{d}{2}} \underbrace{\exp(-tm^2)}_{\leq 1} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}\right) dt \leq \int_0^\infty t^{-\frac{d}{2}} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}\right) dt$$

the inequality in eq. 7.23 is readily demonstrated.

### 7.2.2 Analysis of the XY contribution and final results for $\rho_{s,2}$

The final point of the above analysis is that in a very good approximation the superfluid density for the system is determined by that of a three-dimensional XY model, defined by the following Euclidean Lagrangian<sup>12</sup>:

$$\mathcal{L}_{\text{XY}} = \frac{|\Delta_0^s|^2}{24\pi M} \eta^{\mu\nu} \partial_\mu \phi \partial_\nu \phi \quad (7.26)$$

with partition function  $Z = \int \mathcal{D}\phi e^{-\int d^3x \mathcal{L}_{\text{XY}}}$ , the  $2\pi$ -periodicity for the angular variable  $\phi$  being understood. The model can be equivalently described by switching to the hamiltonian formalism on a discrete lattice as follows:

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \quad (\text{isotropic case})$$

$$H = -J_z \sum_i \cos(\theta_i - \theta_{i+\hat{z}}) - J_{xy} \sum_i \sum_{\mu=\hat{x},\hat{y}} \cos(\theta_i - \theta_{i+\mu}) \quad (z\text{-anisotropic case})$$

for an opportune choice of the coupling constants  $J_i$ , this latter notation being more customary in literature. It is important noting that, as clear

<sup>12</sup>We drop the  $s$  subscript for the phase in this section.

from eq. 7.26, that the imaginary time component now plays the same role as the two spatial components, and the analogue of inverse temperature is defined by the coupling constant  $\frac{|\Delta_0^s|^2}{24\pi M}$ . It is clearly seen that the behaviour of the model is not altered from a qualitative point of view, because the coupling constant is a monotonically decreasing function of temperature as is  $\beta$ : we then have that the low-temperature and high-temperature phases are not mixed or switched, however the transition between the two is now determined by  $|\Delta_0^s|^2$ . We can give an estimate for the critical value  $|\Delta_0^s|_c^2$  as follows, by writing down the condition for which the system is at the critical point:

$$\left(\frac{|\Delta_0^s|_c^2}{24\pi M}\right)^{-1} = T_c^{3DXY} \quad (7.27)$$

$T_{3DXY}^c$  being the critical temperature for the A3DXY model; we tentatively impose  $T_{3DXY}^c \approx 2.2021$  which is the critical temperature for the isotropic case, and this choice will be justified by noting that  $|\Delta_0^s|_c^2$  is substantially independent from the critical temperature. In order to show that one can solve eq. 7.27 for  $|\Delta_0^s|^2$ , recalling that  $M = \sqrt{m_s^2 - 2|\Delta_0^s|^2}$  obtaining:

$$\left(\frac{24\pi}{T_c^{3DXY}}\right)^2 \left(m_s^2 - 2|\Delta_0^s|_c^2\right) = |\Delta_0^s|_c^4$$

the only physical (i.e. real and positive) solution being  $|\Delta_0^s|_c^2 \approx \frac{m_s^2}{2} + O\left(\frac{m_s^4}{576\pi^2 T_c^2}\right)$ , so that at leading order the critical temperature does not contribute to determining  $|\Delta_0^s|_c^2$ . It is then convenient defining an effective temperature  $\Theta$  for the A3DXY model, which is only indirectly related to the real temperature of the system by means of its defining relation  $\Theta = \frac{24\pi M}{|\Delta_0^s|^2}$ ; a plot of the relation<sup>13</sup> between the real temperature  $T$  and the effective temperature  $\Theta$  is given in fig. 7.2.

<sup>13</sup>Up to an irrelevant global constant.



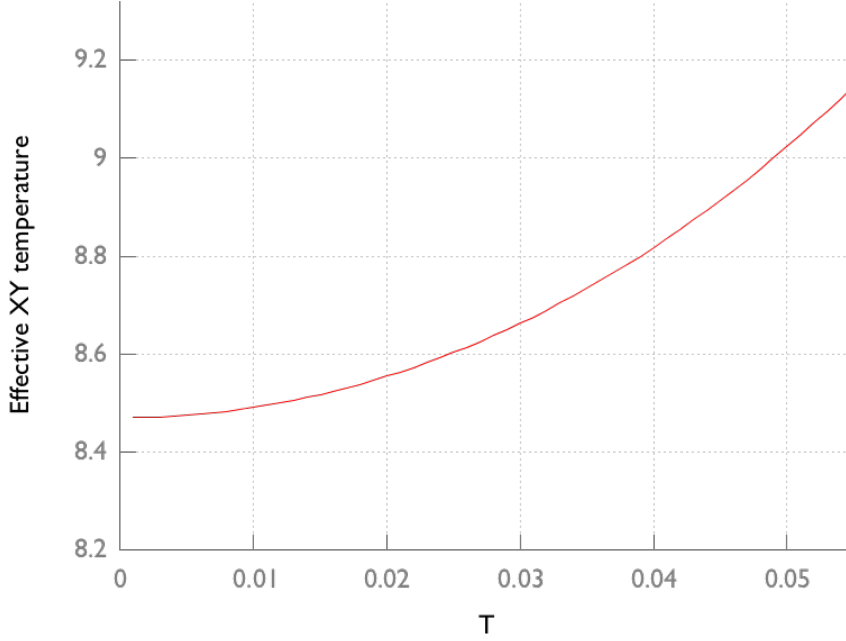


Figure 7.2: The relation between the real and effective temperature, in the range  $[0, T_c]$ , calculated for  $\delta = 0.12$ ; the qualitative behaviour is not altered for different doping values.

In studying the superfluid density we are interested only in the region for which  $\rho_s \neq 0$ , i.e. the region below the critical temperature; clearly  $\Theta_c = \frac{24\pi M}{|\Delta_0^s|_c^2} \approx 2.2021$  but the effective temperature is not allowed to go to zero, its minimum value being:  $\Theta_{\min} = \frac{24\pi M}{|\Delta_0^s|_{\max}^2}$  when  $T = 0$  because, as clearly seen from the plot of the numerical solution for the spinon gap equation in fig. 6.3,  $|\Delta_0^s|^2$  reaches its maximum value for  $T = 0$ .

The superfluid density will be then the one of a three-dimensional XY model constrained in the temperature range  $[\Theta_{\min}, \Theta_c]$  as defined above. Also the correspondence between the real temperature range  $[T = 0, T_c]$  and the effective temperature range  $[\Theta_{\min}, \Theta_c]$  is not linear but has good enough features to preserve two key features of the 3DXY model, namely:

- The map  $\Theta(T)$  is non-singular for  $T = T_c$ , so that the critical exponent

for superfluid density is preserved.

- The map is also (slowly) linearly increasing for low temperatures, so that, at least partially, the low-temperature linearity should be preserved as well.

As main result of the present thesis we can now calculate and plot the superfluid density as a function of the temperature (fig. 7.3); all the quantities related to the XY model have been calculated with a Montecarlo simulation on a  $20 \times 20 \times 20$  lattice with periodic boundary conditions; a cluster update strategy (the so-called Wolff algorithm, [44]) has been used in order to prevent critical slowing. The other quantities (e.g.  $\rho_{s,0}$ ) have been calculated numerically or analytically when a closed-form expression was available.

In addition to that we note that the results of quantities calculated in the present model could be affected by the MFA introduced in chapter 6, especially for very low temperatures; the same phenomenon can be observed, for instance, in [7] where the shape of the phase diagram for cuprates is reproduced in a very reasonable agreement with experimental data, except for an area below a certain temperature, where only a qualitative agreement can be observed. For these reasons we give in fig. 7.4 another plot of superfluid density where the very low- $T$  behaviour has been linearly extrapolated from higher temperatures, in the  $[0, \frac{T_c}{5}]$  range. The physical soundness of the procedure just described can also be verified by noting that the very small slope observed in  $\rho_s(T)$  is a consequence of the flatness of  $\Theta(T)$ , which, in turn, depends upon  $\Delta_0^s(T)$ . The slope of  $\Delta_0^s(T)$  at very low temperatures is not an essential feature of the model in [7] and is affected by the choice of parameters; this reinforces our previous statement about the validity of very low- $T$  predictions of the present model, and further justifies the linear extrapolation presented in fig. 7.4.

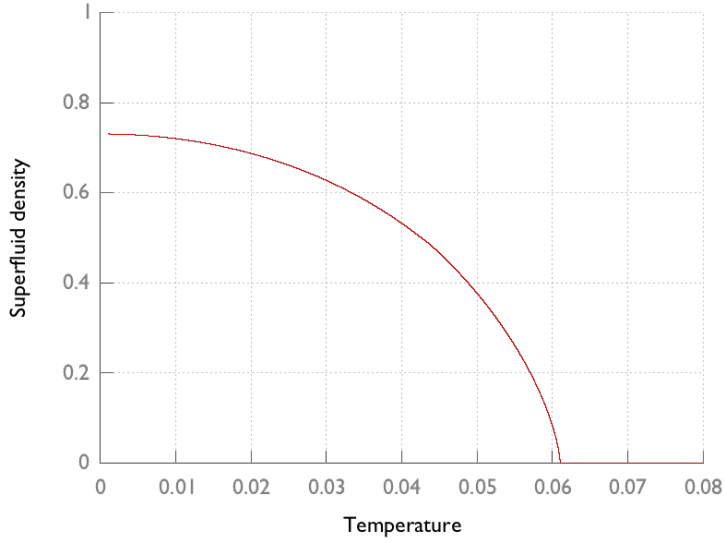


Figure 7.3: The contribution to superfluid density coming from  $S_{\text{eff}}^{s,2}$ . Both in the  $x$  and the  $y$  axis arbitrary units are used, the doping has been set to  $\delta = 0.12$ .

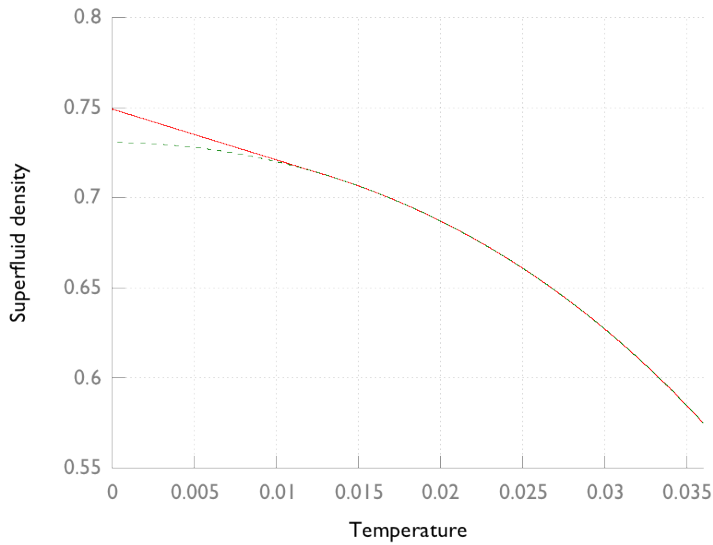


Figure 7.4: The contribution to superfluid density coming from  $S_{\text{eff}}^{s,2}$ , calculated with the same parameters as in in fig. 7.3; for temperatures below  $\frac{T_c}{5}$  a linear extrapolation has been used. The dashed curve shows the “unmodified” superfluid density, as in fig. 7.3. Only the low-temperature region has been plotted, i.e. the region where the two plots actually differ.

### 7.3 Final results and comparison with experimental data

We now compare our results with the experimental data, as reported in section 2.7; as already noted in the introduction of the present chapter, we recall that the contribution for  $S_{\text{eff}}^{s,0}$  and  $S_{\text{eff}}^{s,2}$  yield different contributions to superfluid density, respectively  $\rho_{s,0}$  which contributes only to mechanically-defined superfluid density and  $\rho_{s,2}$  which contributes both to electromagnetically-defined and mechanically-defined superfluid density. This dichotomy is a peculiarity of the present model, and is not present in theories of conventional superconductivity or in the majority of theories for high-temperature superconductivity. As all the experiments known to the author at the time of writing deal with  $\rho_s^{\text{EM}}$ , we must compare  $\rho_{s,2}$  with experimental data. We then observe that:

- The critical exponent for superfluid density, defined by:

$$\rho_s \sim \left| \frac{T - T_c}{T_c} \right|^\delta \quad \text{for } T \rightarrow T_c \quad (7.28)$$

is exactly reproduced to be the one of a 3DXY model, i.e.  $\delta \approx 0.66$ , and indeed correspond to the fact that the superconducting transition is defined by eq. 6.10 which is essentially a 3DXY model; this result is in very good agreement with experimental data, as analyzed in section 2.7.

- On the other hand the low-temperature linearity, i.e.

$$\rho_s \sim 1 - \alpha T \quad \text{for } T \rightarrow 0 \quad (7.29)$$

is reproduced by the model used in the present thesis down to quite low temperatures, but the slope of  $\rho_s(T)$  flattens as  $T \rightarrow 0$ ; this fact

can be explained referring to the discussion of the validity of the MFA approximation for very low temperatures in subsection 7.2.2. An *a posteriori* linear extrapolation for very low temperatures, thoroughly justified in subsection 7.2.2, shows, indeed, a very good agreement with all the general features superfluid density in cuprate.

- We have also been able to reproduce the Uemura relation, i.e. the observation originally made by Uemura and coworkers that in the underdoped regime the following linearity relation holds

$$T_c \propto \rho_s(T = 0)$$

as the doping is varied. This empirical law can be verified by calculating the superfluid density for various dopings, in the underdoped regime, and then drawing a straight line connecting, for every  $\rho_s$  curve, the  $x$ -axis intercept and the  $y$ -axis intercept. It is clearly seen that the Uemura relation is equivalent to requiring that the slopes of those lines should be constant when the doping is varied; the reader can refer to 7.6. A comparison of fig. 7.5 and fig. 7.7 immediately shows that the linearity is reproduced quite accurately.

We also note that, should an experiment be able to measure<sup>14</sup>  $\rho_s^F$  the observed superfluid density should be given by the sum of the contributions in fig. 7.1 and in fig. 7.3. Consequently a high-temperature tail extending beyond  $T_c$  and up to  $T_{ps}$  should be observed according to the model used throughout this thesis. This unique feature is a direct consequence of spin-charge separation and of the fact the superconductivity is achieved in three different steps.

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<sup>14</sup>We do not discuss here the technical feasibility of such a measure.

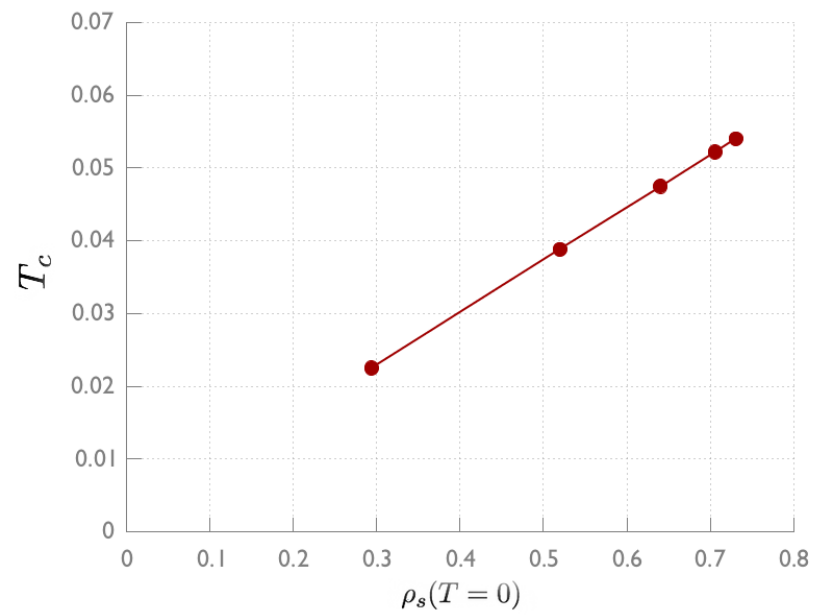


Figure 7.5: The Uemura plot as derived from the model used in the present thesis: each point in the graph corresponds to different doping value, following the line from left to right they are from  $\delta = 0.095$  to  $\delta = 0.12$  at 0.005 steps. Both in the  $x$  and the  $y$  axis arbitrary units are used.

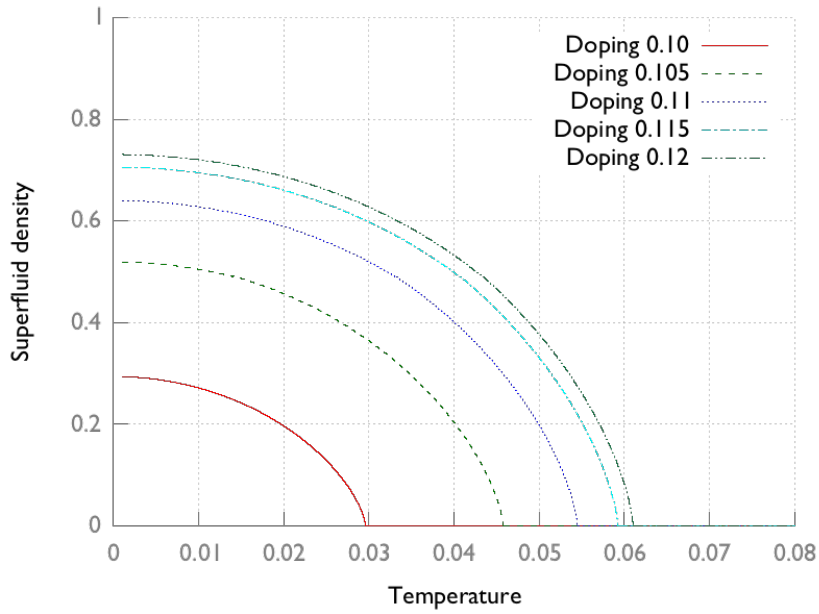


Figure 7.6:  $\rho_{s,2}$  (no linear extrapolation is used for low  $T$ s) as a function of the temperature for various doping values in the underdoped regime.

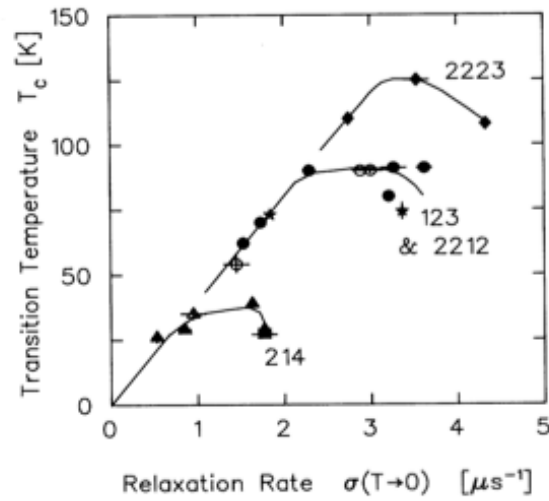


Figure 7.7: The Uemura plot as presented in [45]. Each different symbol type corresponds to a different cuprate compounds, doping is increased for identical compound going from left to right. The relaxation rate  $\sigma(T=0)$  is  $\propto \rho_s(T=0)$





## Chapter 8

# Conclusion and future developments

We sum up the results of the present thesis: we were able to demonstrate that the model used in this thesis is able to correctly reproduce some essential features of superfluid density in cuprates, namely:

- The critical exponent of the superfluid density, which turns out to be exactly the one of a three-dimensional XY model.
- The Uemura relation, i.e. a linear relation between the zero-temperature superfluid density and the critical temperature at which superconductivity ensues, holding for a wide range of dopings in the underdoped regime.

The very low-temperature behaviour of superfluid density, on the other hand, is not exactly reproduced due to the MFAs used which are not as accurate for very low temperatures. An extrapolation procedure which yields correct results even for very low temperatures has been proposed, justified and thoroughly discussed.

As a result of the present thesis we also conjecture that, as opposed to BCS superconductors, the difference between  $\rho_s^F$  and  $\rho_s^{EM}$  should be ob-

servable in cuprates: usually in experiments the electromagnetically-defined superfluid density is measured; we propose that in an experiment sensitive to the mechanically-defined superfluid density a different behaviour should be observed, with a non-zero superfluid density extending even in a range of temperature above  $T_c$ .

As far as future developments are concerned we note that, being the present thesis based on the model introduced in [7], it is consequently consistent with the parameters choice used by authors of the paper; one could try tuning the parameters of the model in a different way in order to see if the accordance of  $\rho_s$  with experimental data could be improved. In particular the low-temperature flat behaviour of  $\rho_s$  does not seem to be an essential feature of the model. However, in doing that great care should be taken in order to retain the correctness of other physical features (e.g. the phase diagram).

## Chapter 9

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# Appendix A

The term  $\frac{p_2^2}{2\mu^2 p^2}$  in  $(L^{-1})^{11}$  gives a contribution to  $W[J]$  (and to the partition function) which is proportional to:

$$\int d^3x \int d^3y \int \frac{d^3k}{(2\pi)^3} \frac{k_2^2}{k^2} e^{ik(x-y)}$$

where it is understood that the integration over  $x$  and  $y$  is performed over a domain  $D$  characterized by a small-distances cutoff, the exact value of the cutoff does not matter for the aims of the present discussion. By means of the same techniques used in section 7.2, starting from eq. 7.20, one can perform the integration of the 0 component of each one of the three integrals, obtaining:

$$\beta \int d^2x \int d^2y \int \frac{d^2k}{(2\pi)^2} \frac{k_2^2}{k_1^2 + k_2^2} e^{ik(x-y)}$$

and the small-distances cutoff just discussed can be made explicit by changing the spatial integration variables:

$$\beta \int d^2(x+y) \int_D d^2(x-y) \int \frac{d^2k}{(2\pi)^2} \frac{k_2^2}{k_1^2 + k_2^2} e^{ik(x-y)}$$

By evaluating the Fourier transform in the innermost integral one obtains:

$$\beta \int d^2u \int_D d^2v \left[ 2\pi\delta^{(2)}(\mathbf{v}) + \frac{-(v_1)^2 + (v_2)^2}{|\mathbf{v}|^4} (\theta(v_1) + \theta(-v_1)) \right] \quad (\text{A.1})$$

with  $\mathbf{u} \equiv \mathbf{x} + \mathbf{y}$ ,  $\mathbf{v} \equiv \mathbf{x} - \mathbf{y}$  and with  $\theta(\#)$  denoting the Heaviside step function. The small-distances cutoff is fundamental in the final evaluation of the integral; clearly it makes the integration avoid the origin so that the Dirac's  $\delta(\#)$  does not yield any contribution and it also allows us to replace the sum of the two step functions with 1. Moreover by noting the the only singularity in the integrand of the remaining part is avoided, again thanks to the domain definition:

$$\int_D dv_1 dv_2 \left[ -\frac{v_1^2}{(v_1^2 + v_2^2)^2} + \frac{v_2^2}{(v_1^2 + v_2^2)^2} \right]$$

it is easily seen that by swapping the dummy  $v_1$  and  $v_2$  variables in the second term the two terms cancel themselves out. That concludes our demonstration.

## Appendix B

# Calculation of the interaction integral

In this appendix we calculate the interaction integral, whose result has been given without demonstration in eq. 7.22. The integral can be written as:

$$\begin{aligned} I &= \int_0^1 dx_1 \int_0^1 dy_1 \int_0^1 dx_2 \int_0^1 dy_2 \ln \left( \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \right) = \\ &= \frac{1}{2} \int_{[0,1]^4} dx_1 dy_1 dx_2 dy_2 \ln \left( (x_1 - x_2)^2 + (y_1 - y_2)^2 \right) \end{aligned}$$

Now we use following variable change:

$$\begin{cases} u = \frac{\sqrt{2}}{2} \frac{x-y}{2} \\ v = \frac{\sqrt{2}}{2} \frac{1+x+y}{2} \end{cases}$$

which also implies that the integration domain must be modified as follows:

$$\int_0^1 dx \int_0^1 dy \longrightarrow \int_{-\frac{\sqrt{2}}{2}}^{\frac{\sqrt{2}}{2}} du \int_{-\frac{\sqrt{2}}{2}+|u|}^{\frac{\sqrt{2}}{2}-|u|} dv$$

The geometrical meaning of the variable and integration domain change is clear by looking at fig. B.1. Using the substitution two times in the integral for  $I$ , as follows:

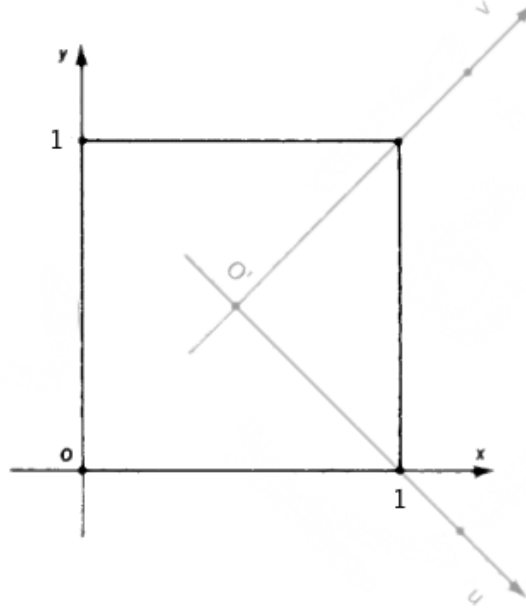


Figure B.1: The variable change as explained in the text,  $O$  being the old coordinate system and  $O'$ , in gray, being the new one.

$$\begin{cases} \alpha = \frac{\sqrt{2}}{2} (x_1 - x_2) \\ \beta = \frac{\sqrt{2}}{2} (1 + x_1 + x_2) \\ \gamma = \frac{\sqrt{2}}{2} (y_1 - y_2) \\ \delta = \frac{\sqrt{2}}{2} (1 + y_1 + y_2) \end{cases}$$

it can be rewritten as:

$$I = \frac{1}{2} \int_{-\frac{\sqrt{2}}{2}}^{+\frac{\sqrt{2}}{2}} d\alpha \int_{-\frac{\sqrt{2}}{2}+|\alpha|}^{+\frac{\sqrt{2}}{2}-|\alpha|} d\beta \int_{-\frac{\sqrt{2}}{2}}^{+\frac{\sqrt{2}}{2}} d\gamma \int_{-\frac{\sqrt{2}}{2}+|\gamma|}^{+\frac{\sqrt{2}}{2}-|\gamma|} d\delta \ln(2\alpha^2 + 2\gamma^2) =$$

$$= 8 \int_0^{\frac{\sqrt{2}}{2}} d\alpha \int_0^{\frac{\sqrt{2}}{2}} d\gamma \left( \frac{\sqrt{2}}{2} - |\alpha| \right) \left( \frac{\sqrt{2}}{2} - |\gamma| \right) \ln(2\alpha^2 + 2\gamma^2)$$

By rescaling the integration variables ( $\alpha \rightarrow \frac{\alpha}{\sqrt{2}}$ ,  $\gamma \rightarrow \frac{\gamma}{\sqrt{2}}$ ) the integral becomes:

$$\begin{aligned} I &= 8 \left( \frac{1}{\sqrt{2}} \right)^2 \int_0^1 d\alpha \int_0^1 d\gamma \left( \frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2}\alpha \right) \left( \frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2}\gamma \right) \ln(\alpha^2 + \gamma^2) = \\ &= 2 \int_0^1 d\alpha \int_0^1 d\gamma (1 - \alpha)(1 - \gamma) \ln(\alpha^2 + \gamma^2) \end{aligned}$$

Switching to polar coordinates:

$$\begin{cases} \alpha = \rho \cos(\theta) \\ \gamma = \rho \sin(\theta) \end{cases}$$

the integral for  $I$  now reads:

$$I = 4 \int_0^{\frac{\pi}{2}} d\theta \int_0^{f(\theta)} \rho d\rho (1 - \rho \cos(\theta))(1 - \rho \sin(\theta)) \ln(\rho)$$

where  $f(\theta)$  is a function which determines the area of integration, which is  $[0, 1]^2$ , i.e. a  $1 \times 1$  square:

$$f(\theta) = \begin{cases} \sqrt{\tan^2(\theta) + 1} & \text{if } 0 \leq \theta \leq \frac{\pi}{4} \\ \sqrt{\tan^2(\theta - \frac{\pi}{2}) + 1} & \text{if } \frac{\pi}{4} < \theta \leq \frac{\pi}{2} \end{cases}$$

In order to carry out the integrals above we note that they are all in the form  $\int x^n \ln(x) dx$ , which can be integrated by parts obtaining:

$$\int x^n \ln(x) dx = \frac{1}{n+1} x^{n+1} \ln(x) - \frac{1}{(n+1)^2} x^{n+1} + C \quad (\text{B.1})$$

The identity above can also be easily verified by direct calculation. We then define  $I_n^\rho = \int \rho^n \ln(\rho) d\rho$  such that:

$$I = 4 \int_0^{\frac{\pi}{2}} d\theta (I_1^\rho - (\cos(\theta) + \sin(\theta)) I_2^\rho + \cos(\theta) \sin(\theta) I_3^\rho |f(\theta)$$

and the integrals can now be performed by using eq. B.1, yielding as a result:

$$\begin{cases} I_1 = \frac{f^2(\theta) \ln(f(\theta))}{2} - \frac{f^2(\theta)}{4} \\ I_2 = \frac{f^3(\theta) \ln(f(\theta))}{3} - \frac{f^3(\theta)}{9} \\ I_3 = \frac{f^3(\theta) \ln(f(\theta))}{4} - \frac{f^3(\theta)}{16} \end{cases}$$

so that:

$$I = 4 \int_0^{2\pi} d\theta (I_1 - I_2 \cos(\theta) \sin(\theta) + I_3 \cos(\theta) \sin(\theta)) \equiv 4 \int_0^{2\pi} d\theta (J_1 + J_2 + J_3)$$

Even these integrals can be evaluated analytically, although the calculation is very lengthy; the results are given in the table below:

	Primitive in the interval $\theta \in [0, \frac{\pi}{4}]$
$J_1$	$\frac{1}{4} (2\theta - 2 \tan \theta + \log(\sec^2(\theta)) \tan(\theta)) - \tan(\frac{\theta}{4})$
$J_2$	$A + \frac{1}{18}  \sec(\theta)  (\sec(\theta) + \sin(\theta))$
$J_3$	$B - \frac{1}{32} \sec^2(\theta)$
	Primitive in the interval $\theta \in [\frac{\pi}{4}, \frac{\pi}{2}]$
$J_1$	$\frac{1}{4} (2\theta - 2 \cot \theta + \log(\csc^2(\theta)) \cot(\theta)) - \cot(\frac{\theta}{4})$
$J_2$	$C + \frac{1}{18}  \csc(\theta)  (\csc(\theta) + \cos(\theta))$
$J_3$	$\frac{1}{16} (\csc^2(\theta) - \csc^2(\theta) \log(\csc^2(\theta))) + \frac{1}{32} \cot^2(\theta)$
A	$-1 + 2\theta + 2\theta \cos(2\theta) + \log(\sec^2(\theta)) + (-2 + \log(\sec^2(\theta))) \sin(2\theta)$
B	$\frac{1}{16} (-\sec^2(\theta) + \log(\sec^2(\theta))) \sec^2(\theta)$
C	$-\frac{1}{12}  \csc(\theta) ^3 \sin(\theta)^2 [4 \cos(\theta) + \csc(\theta) + 4\theta \sin(\theta) + \csc(\theta) \log(\csc^2(\theta)) (\cos(\theta) + \sin(\theta))^2]$



and by evaluating the primitives at  $\theta = \frac{\pi}{2}$  and  $\theta = 0$  one gets the final result which is:

$$I = -\frac{-25 + 4\pi + 2 \log(4)}{12} \approx 0,805$$

as anticipated in eq. 7.22.