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Effects of a *strict* site-occupation constraint in the description of quantum spin systems at finite temperature

Thèse

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Abstract

We study quantum spin systems described by Heisenberg-like models at finite temperature with a strict site-occupation constraint imposed by a procedure originally proposed by V. N. Popov and S. A. Fedotov [66]. We show that the strict site-occupation constraint modifies quantitatively the behaviour of physical quantities when compared to the case for which this constraint is fixed in the average by means of a Lagrange multiplier method. The relevance of the Néel state with the strict site-occupation contraint of the spin lattice is studied. With an exact site-occupation the transition temperature of the antiferromagnetic Néel and spin liquid order parameters are twice as large as the critical temperature one gets with an average Lagrange multiplier method. We consider also a mapping of the low-energy spin Hamiltonian into a QED_3 Lagrangian of spinons. In this framework we compare the dynamically generated mass to the one obtained by means of an average site-occupation constraint.

Résumé

Nous étudions des systèmes de spin quantiques à température finie avec une contrainte d'occupation stricte des sites au moyen d'une procédure introduite par V. N. Popov et S. A. Fedotov [66]. Nous montrons que cette contrainte modifie le comportement d'observables physiques par rapport au cas où cette contrainte est fixée de façon moyenne par la méthode des multiplicateurs de Lagrange. La pertinence de l'état de Néel est étudiée en présence de la contrainte stricte d'occupation des sites du réseau de spin. La température de transition des paramètres d'ordre antiferromagnétique de Néel et d'état de liquide de spins sont doublés par rapport à ceux obtenu par la méthode moyenne des multiplicateurs de Lagrange. Nous considérons l'Hamiltonien de basse énergie décrit par un Lagrangien de QED_3 pour les spinons. Dans ce contexte la masse générée dynamiquement est comparée à celle obtenue par la méthode d'occupation moyenne de site.

à mes parents Huguette et Bertrand
à mon frère Vivien

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Contents

Chapter 1

Résumé

1.1 La procédure de Popov et Fedotov (PFP)

Après la découverte de la supraconductivité par Bednorz et Müller [10] un effort théorique important fut consacré à la recherche d'une explication à ce phénomène qui se manifeste à une température critique élevée. De nombreux supraconducteurs furent découverts parmi lesquels on retrouve les cuprates avec $La_{2-x}Sr_xCuO_4$ et $Bi_2Sr_2CaCu_2O_8$ qui sont des exemples de supraconducteurs dopés en trous, les ruthénates Sr_2RuO_4, les métaux à fermions-lourds tels que UPt_3 et $ZrZn_2$, ainsi que les matériaux organiques comme $\kappa - (BEDT - TTF)_2 - Cu[N(CN)_2]Br$.

Tous les cuprates partagent la même structure atomique composée de couches de CuO_2, tenues pour responsables de la formation de paires de Cooper et de la supraconductivité, et intercalées de couches de substance dopante et/ou non-dopante.

Dans ce manuscrit nous nous concentrerons sur les couches CuO_2 et plus précisement sur la phase isolante antiferromagnétique des supraconducteurs haute température. En effet, la phase isolante des matériaux comme les cuprates peut être modélisée par le modèle de Heisenberg.

L'étude de la phase isolante est motivée par le fait que les corrélations sous-jacentes à la phase antiferromagnétique isolante pourrait se prolonger dans la phase supraconductrice sous l'effet du dopage. En d'autre termes nous attendons que la phase supraconductrice garde quelques traits de caractère de la phase antiferromagnétique isolante.

Notre travail est centré sur l'étude des effets de la contrainte stricte d'occupation de site de spin caractérisant la phase isolante dans la description de système de spin quantique à température finie. Cette contrainte consiste à imposer exactement un spin $S = 1/2$ pour chaque site de réseaux.

L'implémentation d'une telle contrainte fut introduite par Popov et Fedotov [66]. Contrairement à d'autre méthodes basées sur l'utilisation de multiplicateurs de Lagrange [7, 8, 71], conduisant à une occupation moyenne, la **p**rocédure de **P**opov et **F**edotov (**PFP**) évite ce traitement approximatif au moyen de l'introduction d'un potentiel chimique imaginaire. Nous portons notre intérêt à l'analyse et l'application de la PFP sur des systèmes antiferromagnétiques de spins à température finie, et nous la comparons aux résultats obtenus par la méthode des multiplicateurs de Lagrange.

1.2 Propriétés magnétiques du modèle de Heisenberg par la PFP

Le chapitre 4 présente et discute l'application du champ moyen et du développement en nombre de boucles pour la détermination de propriétées physique de systèmes antiferromagnétique de type Heisenberg pour des dimensions D du réseau [21].

Des travaux récents sur des systèmes de spins quantiques discutent l'existence possible d'états de liquide de spin, et pour deux dimensions d'espace de la compétition ou transition de phase entre états liquide de spin et antiferromgnétique de Néel [28, 57, 74, 75]. Il est également connu que les supraconducteurs (cuprates) présentent une phase antiferromagnétique [50].

Dans le chapitre 4 nous focalisons notre attention sur la phase dont le champ moyen est de type Néel dans la description des systèmes quantiques de spin représentés par le modèle de Heisenberg. Plus précisément, nous présentons une étude détaillée de l'aimantation et de la susceptibilité magnétique pour ces systèmes de réseaux de spin en dimension D et à température finie. Le but de ce travail est d'étudier la pertinence de l'*ansatz* de Néel comme approximation de champ moyen en utilisant la PFP et pour les intervalles de températures $0 < T < T_c$ où T_c est la température critique. Dans l'objectif d'obtenir une réponse sur ce point nous calculons les contributions des fluctuations quantiques et thermiques au-delà de l'approximation de champ moyen et sous la contrainte d'occupation stricte d'un seul spin par site de réseau [9, 21, 22, 42, 66]. Une comparaison est effectuée entre nos résultats et ceux obtenus par la théorie des ondes de spins sur les modèles de Heisenberg et XXZ.

Il est montré que la PFP introduit un grand décalage de la température critique par rapport à celle obtenue par la méthode ordinaire des multiplicateurs de Lagrange. En effet, il apparait un doublement de la température de transition entre un état antiferromagnétique de Néel et la phase paramagnétique [9, 22]. Nous montrons dans le chapitre 4, et c'est là une des contribution originales de ce travail de thèse, qu'à basse température l'aimantation ainsi que la susceptibilité magnétique sont égalles en valeur à celles obtenues par la théorie des ondes de spin, comme le montre la figure 4.3 du chapitre 4. La figure 4.3 représente l'aimantation en champ moyen (en traits tiretés), l'aimantation avec fluctuation en utilisant la PFP (en traits plein) et enfin l'aimantation calculée par la théorie des ondes de spins (en traits pointillés), pour des systèmes tri-dimensionnels. La superposition des courbes à basse température apparait clairement sur cette figure. Le décalage entre l'aimantation moyenne et celle obtenue en considérant les fluctuations est due à l'effet intrinsèque des fluctuations quantiques et thermiques sur la moyenne statistique des orientations de spin. La PFP n'est pas responsable de ce décalage.

À plus haute température les contribution des fluctuations de nature quantiques et thermiques croissent en une singularité au voisinage de la température critique. L'hypothèse que le champ moyen de Néel contribue pour une majeure partie à l'aimantation et à la susceptibilité n'est plus valide. En approchant de la température critique T_c l'aimantation en champ moyen tend vers zéro et les fluctuations croissent de plus en plus à l'ordre d'une boucle. Ceci résulte en une divergence de la valeur théorique prévue pour l'aimantation globale du système de spins. Ce comportement est commun aux modèle de Heisenberg et XXZ. Nous en déduisons que la brisure de symétrie induite par le choix de l'état de Néel n'est pas impliquée dans l'apparition des divergences calculées.

L'influence des fluctuations décroit avec l'augmentation de la dimension D du système due à la réduction des fluctuations par rapport au champ moyen.

En dimension $D = 2$ l'aimantation vérifie effectivement le théorème de Mermin et Wagner [55]. Pour $T \neq 0$, les fluctuations sont plus importantes que la contribution du champ moyen. Ainsi dans une description plus réaliste de la physique il est nécessaire de prendre en considération d'autre champ moyen. En effet, Ghaemi et Senthil [28] ont montré, à l'aide d'un modèle spécifique, qu'une transition du second ordre d'un état de Néel vers un liquide de spins pourrait apparaître en fonction de la valeur des couplages. Ceci nous conduit au chapitre 5 dans lequel une étude de l'influence de la PFP est menée sur différents *ansatz* de champ moyen et pour des réseaux bi-dimensionnels.

Le point originale de ce chapitre 4 est l'utilisation de la procédure de Popov et Fedotov dans la calcul de propriétées magnétique à température finie et pour un ordre à une boucle en perturbation [21].

1.3 Champ moyens pour le modèle bidimensionnel de Heisenberg

Nous résumerons dans cette section le contenu du chapitre 5 où nous considérons la PFP appliquée à des systèmes de spin quantique à température finie. Le but de ce chapitre est de confronter l'approche utilisant la PFP à celle utilisant un multiplicateur de Lagrange pour fixer la contrainte d'occupation par site du réseau de spin.

La description des systèmes quantiques de spins à température finie passe généralement par l'utilisation d'une procédure de *point-selle* qui est une approximation d'ordre zéro de la function de partition. La solution de champ moyen ainsi générée peut fournir une approximation réaliste de la solution exacte.

Cependant, les solutions de champ moyen ainsi obtenue ne sont pas uniques. Le choix d'un bon champ moyen repose essentiellement sur les propriétées du système considéré, en particulier sur ses symétries. Ceci génère des difficultés majeures. Une quantité considérable de travail à été fait sur ce point et il y a une littérature importante sur le sujet. En particulier, les systèmes qui sont bien décrits par des modèles de type Heisenberg sans frustration semblent , selon leur dimension, bien compris par l'introduction de l'état ferromagnétique ou antiferromagnétique de Néel à température nulle $T = 0$ [13, 12]. Cependant il n'en n'est pas de même pour beaucoup de systèmes de basse dimensionnalité ($D \leq 2$) et/ou frustrés [82, 56, 47]. Ces systèmes présentent des caractéristiques spécifiques. Une analyse extensive et une discussion, pour des dimensions $D = 2$, ont été présentées par Wen [80]. La compétition entre état antiferromagnétique et liquide de spins ont fait l'objet de récentes investigations dans le cadre de la théorie quantique des champs à température nulle [78, 34].

La raison de ces comportements spécifiques des systèmes de basse dimension peut être qualitativement relié au fait que les fluctuation quantiques et thermiques sont très fortes, et détruisent ainsi l'ordre antiferromagnétique. Ceci motive une transcription de l'Hamiltonian en termes d'opérateurs composés que nous appelons “diffuson” et “coopéron”.

Le chapitre 5 compare le traitement exact (obtenue par la PFP) et moyen (par un multiplicateurs de Lagrange) de la contrainte d'occupation pour différentes approches de l'Hamiltonien de Heisenberg.

En résumé, nous montrons au chapitre 5 que la contrainte stricte d'occupation induit une différence quantitative de la température critique en la comparant avec les résultats obtenus par une contrainte d'occupation moyenne. En conséquence il apparait un effet mesurable sur le comportement des paramètres d'ordre. C'est là encore un point original de cette thèse qui à conduit à l'article donné en réference [22].

Avec l'occupation exacte de spin, la température de transition des états de liquides de spins et antiferromagnétiques de Néel sont le double de la température critique obtenue par la méthode des multiplicateurs de Lagrange.

En revanche, la PFP ne peut pas être employée dans une description en terme de "coopérons". Les coopérons sont à considérer comme des paires BCS et détruisent ainsi deux quasi-particules en faveur de la création d'une nouvelle qui n'est autre qu'une paire du type BCS. Il en résulte que dans ce cas le nombre de particules n'est pas conservée au contraire de la contrainte exacte. Or il se trouve que la PFP ne tolère aucune fluctuation du nombre de particule.

Dans une description plus réaliste nous devons tenir compte des contributions des fluctuations quantiques et thermiques qui peuvent être d'une importance cruciale en particulier au voisinage des points critiques. Le chapitre 6 se consacre à l'implication des fluctuations de phase autour du champ moyen dans l'état π-flux.

1.4 Du modèle de Heisenberg à l'action QED_3 pour des température finie

Un ansatz de Néel n'est pas nécessairement un bon candidat pour la description des systèmes de spin quantique a deux dimensions. Nous avons montré au chapitre 4 qu'un tel ansatz brise la symétrie $SU(2)$ générant les bosons de Goldstone qui détruisent l'ordre de Néel. Un meilleur candidat semble être le liquide de spins étant donné qu'il conserve la symétrie $SU(2)$ intacte. Pour cette raison, le chapitre 6 se concentre sur la phase liquide de spins.

L'Électrodynamique Quantique à deux dimensions d'espace et une de temps , la QED_3, est un cadre commun qui peut être utilisé pour décrire les systèmes fortement corrélés aussi bien que les phénomènes spécifiques qui y sont reliés comme la supraconductivité à haute température [27, 28, 50, 57]. Une formulation en théorie des champs du modèle de Heisenberg en $D = 2$ dimensions d'espace fait correspondre l'action initiale à une action QED_3 pour les spinons [28, 57]. Avec cette description apparait le problème du champ moyen et les questions corrélées au confinement des charges tests qui peuvent conduire à l'impossibilité de déterminer les contributions des fluctuations quantiques au travers de développements en nombre de boucles [32, 33, 62].

Nous considérons dans le chapitre 6 l'état π-flux initialement introduit par Affleck et Marston [2, 54]. L'occupation des spins par site du réseau est toujours fixée par la PFP. La PFP introduit un potentiel chimique imaginaire modifiant les fréquences de Matsubara induisant en retour des modifications perceptibles au niveau de la température de restauration de la symétrie chirale. La symétrie chirale est initialement brisée par la génération dynamique de masse des spinons.

Nous nous concentrons sur la génération et le comportement de la masse des spinons due à la présence du champ de jauge $U(1)$. Appelquist et cie. [5, 6] ont montré qu'à température zéro les fermions initialement sans masse peuvent acquérir une masse générée dynamiquement lorsque le nombre de saveur N est inférieur à la valeur critique $N_c = 32/\pi^2$. Plus tard Maris [52] a confirmé l'existence d'une valeur critique $N_c \simeq 3.3$ au-dessous de laquelle la masse dynamique peut-être générée. Étant donné que nous considérons des spins $S = 1/2$ nous avons $N = 2$ et ainsi $N < N_c$.

À température finie, Dorey et Mavromatos [24] et Lee [48] ont montré que la masse générée dynamiquement s'annule pour une température T plus grande que la valeur critique T_c.

Nous montrons que l'utilisation du potential chimique imaginaire introduit par la PFP [66] modifie notablement le potentiel effectif entre deux particules chargées et double la température critique T_c en accord avec les résultats présentés précédement [22].

Le potentiel chimique imaginaire réduit le phénomène d'écrantage du potentiel d'interaction entre des fermions test losrqu'on le compare à celui obtenu par la méthode des multiplicateurs de Lagrange.

Nous montrons également que la température de transition de la restauration de la symétrie "chirale", où la masse des spinons $m(\beta)$ s'annule, est doublée par le potentiel chimique imaginaire de Popov-Fedotov. Le paramètre d'ordre $r = \frac{2m(0)}{k_B T_c}$ donné par Dorey et Mavromatos [24] et Lee [48] s'en trouve réduit de moitié. La théorie, dans l'état dans lequelle elle est actuellement, ne peut pas rendre compte de la mesure expérimentale de r qui est environ de 8 pour $YBaCuO$.

Tous ces résultats ont donné lieu à l'article cité en référence [23].

1.5 Perspectives

Marston [53] a montré que pour retirer les configurations interdites de la jauge $U(1)$ dans le modèle antiferromagnétique de Heisenberg, un terme de Chern-Simons apparait naturellement et doit être inclus dans l'action QED_3. Cette contrainte supplémentaire conduit à fixer à π (modulo 2π) le flux au travers de la plaquette formée par la maille élémentaire du réseau de spins. De nouveaux travaux, que nous n'avons pas abordés dans ce manuscrit, montrent que la température de transition chirale ainsi que le rapport $r = m/T_c$ peuvent être controlés par le coefficient de Chern-Simons [20].

D'autre points intéressants consernent la compactification du champ de jauge $U(1)$ que nous avons utilisé pour obtenir la masse dynamique des spinons. Dans le cas d'une théorie de jauge compacte des instantons apparaissent et interagissent avec la matière (ici les spinons) et peuvent changer le comportement du système de spin [64, 65]. Le confinement des spinons par les instantons reste un problème ouvert.

Chapter 2

Introduction

After the discovery of high temperature superconductivity by Bednorz and Müller [10] great theoretical efforts were devoted to find an explanation of the mechanism underlying the very high critical temperatures phenomenon. Many new superconductors were discovered amoung which one have cuprates with $La_{2-x}Sr_xCuO_4$ and $Bi_2Sr_2CaCu_2O_8$ are examples of hole doped superconductors, ruthenates Sr_2RuO_4, heavy-fermion metals such as UPt_3 and $ZrZn_2$, and organic materials like the well known $\kappa-(BEDT-TTF)_2-Cu[N(CN)_2]Br$.

In particular cuprates behave differently from the conventional BCS superconductors. Experimentalists observed d-symmetry of the order parameter, strong electronic correlations and non-conventional but "universal" phase diagrams as shown in figure 2.1 [11].

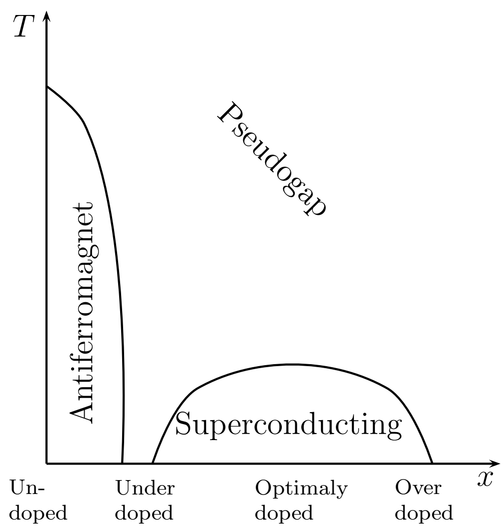


Figure 2.1: Schematic phase diagram of a cuprate as a function of hole doping x and temperature T

All cuprates share the same kind of atomic structure which consists of a layered structure made of CuO_2-layers which are considered as responsible for Cooper-pairing and superconductivity.

In the following we concentrate on the CuO_2 layers and more precisely on the antiferromagnetic insulating phase of the high-T_c superconductors which corresponds to the undoped regime as shown in figure 2.1. The insulating phase of the cuprates like compound, the so called parent compound, can be modelled by Heisenberg models.

The study of the insulating phase is motivated by the fact that under doping the parent compound should keep a *memory* of the correlations underlying the antiferromagnet insulating phase. In other words one believes that the superconducting phase must partially conserve some characters of the antiferromagnet insulating parent compound.

Our work is devoted to the study of the effects of a *strict* site-occupation constraint caracterising the insulating phase in the description of quantum spin systems at finite temperature. This constraint consists in the enforcement of the occupation of each lattice site by exactly one $S = 1/2$ spin. The implementation of such a constraint was introduced by Popov and Fedotov [66]. Contrary to other methods which are based on the use of a Lagrange mutliplier [7, 8, 71] leading to an average occupations the **P**opov and **F**edotov **p**rocedure (**PFP**) avoids this approximate treatment by means of the introduction of an imaginary chemical potential as we will show in chapter 3. We are interested to work out and analyse the application of the PFP onto antiferromagnet spin systems at finite temperature and to compare these results with the Lagrange multiplier method.

Chapter 3 introduces the mathematical tools found in the literature and which will be used throughout this manuscript. We present the fermionization of spin Hamiltonian models and the PFP. We show that the PFP eliminates the *unphysical* Fock states in the fermionization of spin models. Finally we construct a path integral formulation of the partition function in imaginary time and show that the PFP induces a modification of the Matsubara frequencies which characterizes the fermionic propagator.

In chapter 4 we concentrate on a Néel mean-field phase description of quantum spin systems. The possible competition or phase transition between spin liquid states and an antiferromagnetic Néel state which may be expected to describe Heisenberg type systems in two dimensions where discussed recently [28, 57, 74, 75]. We aim to study the pertinence of the Néel state ansatz as a mean-field approximation for finite temperature using the PFP. Quantum and thermal fluctuations contributions are worked out at the one-loop level taking the Popov and Fedotov procedure into account. The outcomes are compared with the spin-wave theory and extended to the XXZ-model by working out the magnetization and the magnetic susceptibility for temperature below and up to critical point. We discuss the degree of realism of the mean-field Néel ansatz. Indeed Ghaemi and Senthil [28] have recently shown, with the help of a specific model, that a second order phase transition from a Néel mean-field to an ASL (algebraic spin liquid) may be at work depending on the strength of interaction parameter which enter the Hamiltonian of the system.

The originality of my work stays here on the fact that magnetic properties have never been worked out using a strict site-occupation constraint. Chapter 4 remedies to it and an article on this point can be found in [21].

In chapter 5 we consider different mean-fields possible choices of quantum spin systems at finite temperature in which each lattice site is occupied by exactly one spin imposed by the PFP. We also construct the formalism in which the occupation constraint is imposed on the average by means of the Lagrange mutliplier method with the aim of confronting these two approaches in the framework of Heisenberg-type models.

The description of strongly interacting quantum spin systems at finite temperature generally relies on a saddle point procedure which is a zeroth order approximation of the partition function. The so generated mean-field solution is aimed to provide a qualitatively realistic approximation of the exact solution. The specific behaviour of low-dimensional systems is characterized by the fact that low-dimensionality induces strong quantum and thermal fluctuations, hence disorder which destroys the antiferromagnet order. This motivates a transcription of the Hamiltonian in terms of composite operators which we call "diffusons" and "cooperons" which are the essence of the well known **R**esonant **V**alence **B**ond (**RVB**) spin liquid states proposed by Anderson [4].

The original point concerns the confrontation of the magnetization obtained through the PFP with the result obtained by means of an average projection procedure in the framework of the mean-field approach characterized by a Néel state. The same confrontation is performed for the order parameter which characterizes the system when its Hamiltonian is written in terms of so called Abrikosov fermions (also called pseudo-fermions or spinons) [22].

Chapter 6 is devoted to a more realistic analysis in which we take care of the contributions of quantum fluctuations which may be of overwhelming importance particularly in the vicinity of critical points.

Quantum Electrodynamics $QED_{(2+1)}$ has attracted considerable interest in the last decade [3, 24, 33, 48, 27] since it is a common framework which can be used to describe strongly correlated systems such as quantum spin systems in 1 time and 2 space dimensions, as well as related specific phenomena like high-T_c superconductivity [27, 28, 50, 57]. A gauge field formulation of antiferromagnetic Heisenberg models in $d = 2$ space dimensions maps the initial action onto a QED_3 action for spinons [28, 57]. We consider the π-flux state approach introduced by Affleck and Marston [2, 54]. The strict site-occupation is introduced by the imaginary chemical potential proposed by Popov and Fedotov [66] for $SU(2)$ spin symmetry which modifies the Matsubara frequencies as will be explained in chapter 3.

We show that at zero temperature the "chiral" symmetry is broken by the generation of a dynamical mass [5, 6] which vanishes at finite temperature T larger than the critical one T_c [24, 48].

We show that the imaginary chemical potential introduced by Popov and Fedotov [66] modifies noticeably the effective potential between two charged particles, doubles the dynamical mass transition temperature T_c and reduces the screening effect of this static potential between test fermions. This last point led to two articles given in [20, 23].

Chapter 7 summarizes and comments our results and suggests further developments aimed to lead to clues to remaining open questions [21, 22, 23].

Chapter 3

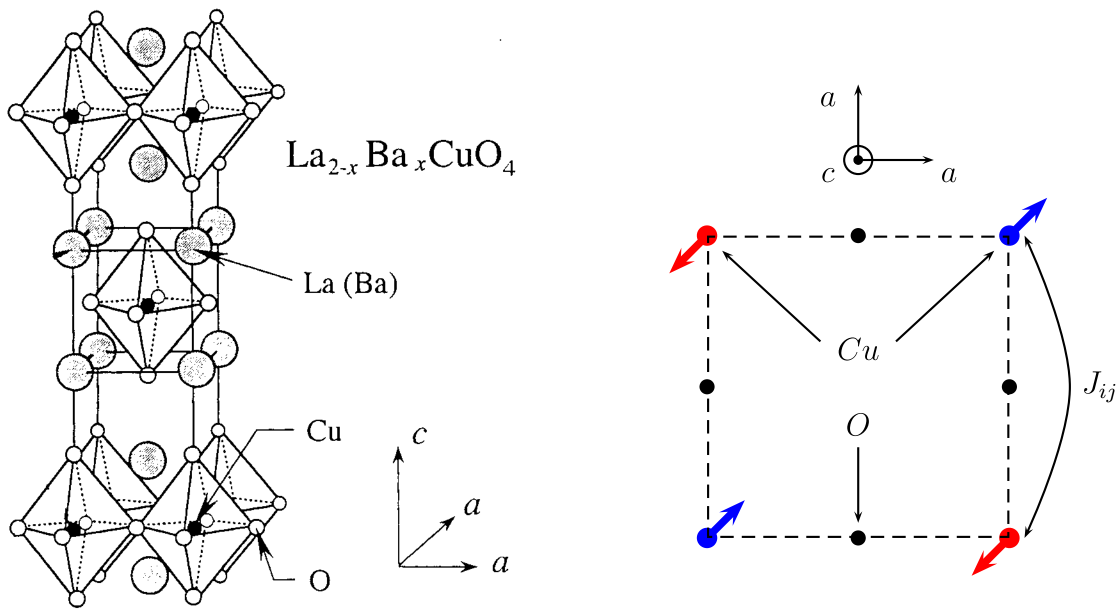
Path integral formulation and the Popov-Fedotov procedure

Contents

We present here a set of technical tools, extracted from literature and mainly taken from Negele and Orland's book [61], which are necessary in order to construct the partition function in terms of a functional integral. The fermionization of a Heisenberg spin-1/2 model is presented. The spin operators are described in the fermionic Fock space by means of the introduction of anticommuting creation and annihilation operators. In order to eliminate the *unphysical* Fock states which correspond to the presence of 0 or 2 particles on each site of the system, we introduce the so-called Popov-Fedotov procedure (PFP). Finally we construct a path integral formulation of the partition function in imaginary time and show that the PFP induces a modification of the Matsubara frequencies which characterize the fermionic propagator.

3.1 Fermionization of spin-1/2 Heisenberg models

Quantum antiferromagnet spin-1/2 models are of great interest for theoretical studies. Indeed they have deep connections with high-temperature superconducting materials such as $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}(Sr \text{ or } Ba)_xCuO_4$ for which the undoped region of the phase diagram shows an antiferromagnetic phase described by a two dimensional square lattice of spin-1/2 particles, as explained in [11, 50]. For example in the parent compound La_2CuO_4 the copper is surrounded by six oxygen atoms forming CuO tetrahedron layers between La layers. Copper atoms interact with each other by means of a superexchange mechanism forming an effective two dimensional square lattice of spin-1/2 as shown in figures 3.1.



(a) (b)

Figure 3.1: (a) Cristallographic structure of the cuprate superconductor $La_{2-x}Ba_xCuO_4$ and (b) a CuO_2 layer showing the (super)exchange coupling between the copper atoms.

In the same direction Dagotto and Rice [18] show that the two-leg spin-1/2 ladder materials, the vanadyl pyrophosphate $(VO)_2P_2O_7$ and the cuprate like $SrCu_2O_3$, can be modelised as a one-dimensional spin-1/2 Heisenberg model.

In order to study these antiferromagnet spin-1/2 systems we will introduce the **H**eisenberg **A**nti-**F**erromagnet **M**odel (**HAFM**) with an external magnetic field $\vec{B}_i$

$$H = -\frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i.\vec{S}_j + \sum_i \vec{B}_i.\vec{S}_i \tag{3.1}$$

where the sums runs over the lattice sites $\vec{r}_i$ and $\vec{r}_j$. The effective (super)exchange coupling J_{ij} (see A.Auerbach [8] chapter 1), acts between spins at position $\vec{r}_i$ and $\vec{r}_j$ on a D-dimensional hypercubic lattice. For antiferromagnet systems J_{ij} is negative and positive in the ferromagnetic case. The second term of the HAFM is the coupling between the spins and the magnetic field $\vec{B}$ at each lattice site $\vec{r}_i$. The *Landé factor* and the *Bohr magneton* coefficients are absorbed in the magnetic field $\vec{B}$.

The spins $\vec{S}$ are vector operators, their components obey a $SU(2)$ Lie algebra $[S_x, S_y] = iS_z$. Here we adopt the convention $\hbar = 1$. The $S = 1/2$ spin vector operators can be expressed using the *Abrikosov* fermionic creation and annihilation operators $f^\dagger_{i\sigma_1}$ and $f_{i\sigma_2}$

$$\vec{S}_i = \frac{1}{2} f^\dagger_{i\sigma_1} \vec{\sigma}_{\sigma_1\sigma_2} f_{i\sigma_2} \tag{3.2}$$

where $\sigma_1, \sigma_2 = \uparrow, \downarrow$ and the $\vec{\sigma}_{\sigma_1\sigma_2}$ vector components are Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.3}$$

Explicitly spin operators at position i read

$$\begin{aligned} S_i^+ &= f^\dagger_{i\uparrow} f_{i\downarrow} && (3.4) \\ S_i^- &= f^\dagger_{i\downarrow} f_{i\uparrow} && (3.5) \\ S_i^z &= \frac{1}{2}(f^\dagger_{i\uparrow} f_{i\uparrow} - f^\dagger_{i\downarrow} f_{i\downarrow}) && (3.6) \end{aligned}$$

The creation and annihilation operators $f_{i\sigma}$ and $f^\dagger_{i\sigma}$ verify the anticommutation relations

$$\begin{aligned} \{f_{i\sigma_1}, f^\dagger_{j\sigma_2}\} &= \delta_{\sigma_1,\sigma_2}\delta_{i,j} && (3.7) \\ \{f_{i\sigma_1}, f_{j\sigma_2}\} &= 0 && (3.8) \\ \{f^\dagger_{i\sigma_1}, f^\dagger_{j\sigma_2}\} &= 0 && (3.9) \end{aligned}$$

Applying (3.4), (3.5) and (3.6) onto the *physical* Fock states $|1,0>$ and $|0,1>$ one gets

$$\begin{aligned} S_i^+|0,1> &= |1,0> \equiv |\uparrow> && (3.10) \\ S_i^-|1,0> &= |0,1> \equiv |\downarrow> && (3.11) \\ S_i^z|1,0> &= -1/2|\uparrow> && (3.12) \\ S_i^z|0,1> &= 1/2|\downarrow> && (3.13) \end{aligned}$$

The insertion of (3.2) into (3.1) generates the Fermionized Heisenberg Antiferromagnet Model which is quartic in the fermion operators. Using this formulation it is possible to write the Hamiltonian in different forms. Indeed the spin interaction term $\vec{S}_i.\vec{S}_j$ can be expressed as

$$\begin{aligned} \vec{S}_i.\vec{S}_j &= \vec{S}_i.\vec{S}_j \\ &= \frac{1}{2}\mathcal{D}^\dagger_{ij}\mathcal{D}_{ij} + \frac{\tilde{n}_i\tilde{n}_j}{4} - \frac{\tilde{n}_i}{2} \\ &= \frac{1}{2}\mathcal{C}^\dagger_{ij}\mathcal{C}_{ij} + \frac{\tilde{n}_i\tilde{n}_j}{4} && (3.14) \end{aligned}$$

where $\tilde{n}_i = \sum_\sigma f^\dagger_{i\sigma} f_{i\sigma}$, $\mathcal{D}$ and $\mathcal{C}$ are quadratic in the fermionic creation and annihilation operators

$$\mathcal{D}_{ij} = f^\dagger_{i\uparrow} f_{j\uparrow} + f^\dagger_{i\downarrow} f_{j\downarrow} \tag{3.15}$$
$$\mathcal{C}_{ij} = f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} \tag{3.16}$$

Néel states, Resonant Valence Bond (RVB) states [4] as well as π-flux states can be introduced by means of (3.14) in order to define different mean-fields, as done by using the large-N method developed by Affleck [1],Affleck and Marston [2] , Read and Sachdev [69, 70, 71].

From equation (3.6) we see that the *physically* acceptable Fock states on a lattice site i are those for which the expectation value of the number operator either $f^\dagger_{i,\uparrow} f_{i,\uparrow}$ or $f^\dagger_{i,\downarrow} f_{i,\downarrow}$ is equal to one an the other equal to zero (corresponding to $< S_z >= \pm 1/2$). The occupation by one fermion per lattice site is fulfilled if

$$\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} = 1 \tag{3.17}$$

One way to implement this constraint consists of the introduction of a projector onto the Fock space using a Lagrange multiplier λ

$$\tilde{P}_i = \int \mathcal{D}\lambda_i e^{\lambda_i (\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} - 1)} \tag{3.18}$$

where λ plays the role of a chemical potential in the framework of the path integral formulation. However such a propagator cannot impose a rigorous constraint (3.17). The actual value of λ is fixed by a saddle point method, that is to say mean-field equations will fix the mean value of the Lagrange parameter. In order to implement the constraint (3.17) in a *strict* way we shall introduce the Popov-Fedotov procedure.

3.2 The Popov-Fedotov procedure (PFP)

The introduction of this procedure is a key point in the present work. In the following we aim to study the consequences of its use in the description of spin systems at finite temperature. In the present section we show how it is able to enforce the constraint (3.17).

The Fock space constructed with the fermionic operators $f, f^\dagger$ is not in bijective correspondence with the Hilbert space of spin states as shown in figure 3.2. Indeed, in Fock space and for spin-1/2 particles, the occupation of each site i can be characterized by the states $|n_{i,\uparrow}, n_{i,\downarrow} >$ with $n_{i,\sigma} \in \{0, 1\}$ the eigenvalue of the occupation operator $f^\dagger_{i\sigma} f_{i\sigma}$, that is the states $|0, 0 >$, $|1, 0 >$, $|0, 1 >$ and $|1, 1 >$. Since the sites have to be occupied by a single particle the *unphysical* states $|0, 0 >$ and $|1, 1 >$ have to be eliminated. This is done by means of a projection procedure proposed by Popov and Fedotov [66] and generalized to $SU(N)$ symmetry by Kiselev *et al.* [42].

Hilbert space		Fock space $\{\vert n_\uparrow, n_\downarrow >\}$
$\vert\uparrow>$	$\Longleftrightarrow$	$\vert 1,0>$
$\vert\downarrow>$	$\Longleftrightarrow$	$\vert 0,1>$
-		$\vert 0,0>$
-		$\vert 1,1>$

Figure 3.2: Correspondance between the Hilbert space and the $S = 1/2$ Fock space

We introduce the projection operator $\tilde{P} = \frac{1}{i^{\tilde{N}}} e^{i\frac{\pi}{2}\tilde{N}}$, where $\tilde{N} = \sum\limits_{i,\sigma} f^\dagger_{i\sigma} f_{i\sigma}$ is the number operator, into the partition function $\mathcal{Z}$ which then reads

$$\mathcal{Z} = Tr\left[e^{-\beta\tilde{H}}\tilde{P}\right] \tag{3.19}$$

where $\tilde{H}$ is the fermionized Hamiltonian of the systems and $\beta = 1/T$ is the inverse temperature, with the convention $k_B = 1$ for the Boltzmann constant. Define the trace of the operator $\mathcal{O}$ in Fock space as

$$Tr\left[\mathcal{O}\right] = \sum_{\{n_{i,\alpha}\in[0,1]\}} \left(\bigotimes_i < n_{i,\uparrow}, n_{i,\downarrow}|\right) \mathcal{O} \left(\bigotimes_i |n_{i,\uparrow}, n_{i,\downarrow} >\right) \tag{3.20}$$

where $\bigotimes\limits_i |n_{i,\uparrow}, n_{i,\downarrow} >$ is the tensor product of the Fock states $|n_{i,\uparrow}, n_{i,\downarrow} >$ for different lattice site i. The contributions of the Hamiltonian should be equal to zero when applied to the *unphysical* states. Since $S_i^+|unphysical >= S_i^-|unphysical >= S_i^z|unphysical >= 0$ all Hamiltonians build with only spin operators $\left\{S_i^+, S_i^-, S_i^z\right\}$ give an energy equal to zero when applied to unphysical states ($H|unphysical >= 0$). The action of $\tilde{P}_j$ on each site j is such that the contributions of states $|0,0>_j$ and $|1,1>_j$ to the partition function $\mathcal{Z}$ eliminate each other. Indeed

$$\begin{aligned} &< 0,0|_j\, e^{-\beta H}.e^{i\frac{\pi}{2}*0}|0,0>_j + < 1,1|_j\, e^{-\beta H}.e^{i\frac{\pi}{2}*2}|1,1>_j \\ &+ < 1,0|_j\, e^{-\beta H}.e^{i\frac{\pi}{2}}|1,0>_j + < 0,1|_j\, e^{-\beta H}.e^{i\frac{\pi}{2}}|0,1>_j \\ &= i\left(< 1,0|_j\, e^{-\beta H}|1,0>_j + < 0,1|_j\, e^{-\beta H}|0,1>_j\right) \end{aligned}$$

Hence the partition function reads

$$\mathcal{Z} = \frac{1}{i^{\mathcal{N}}}.Tr\left[e^{-\beta(\tilde{H}-\mu\tilde{N})}\right] \tag{3.21}$$

where $\mathcal{N}$ is the total number of spin sites in the considered lattice. Equation (3.21) with the *imaginary chemical potential* $\mu = i\frac{\pi}{2\beta}$ describes a system with strictly one fermion (spin-$\uparrow$ or spin-$\downarrow$) per lattice site, in contrast with the usual method which introduces an average projection by means of a real Lagrange multiplier [8, 7].

In the following the Heisenberg model will be studied in the path integral formulation using the Popov-Fedotov procedure. The consequences of its application will be compared to those obtained by means of Lagrange formulations.

3.3 Path integral formulation of the partition function

In the present section we construct the path integral formulation of the partition function (3.21). First we shall define the coherent states of the fermionic Fock space. Then we derive from these states the appropriate properties which lead from the trace of an operator over Fock state into the trace over coherent states of the same Fock space. This leads to the functional integral expression of the partition function (3.21).

3.3.1 Fermionic coherent states

The coherent states are an overcomplete linear combination of the set of states in Fock space. They are eigenstates of the annihilation operator, bosonic as well as fermionic [61].

Define $|\xi>$ as the coherent state of the fermionic Fock space

$$|\xi>=\sum_{k=0}^{\infty}\sum_{\{n_\alpha\}=0}^{1}(-1)^{\sum_\alpha n_\alpha}\,\xi_1^{n_1}\dots\xi_\alpha^{n_\alpha}\dots\xi_k^{n_k}|n_1,\dots,n_\alpha,\dots,n_k> \tag{3.22}$$

where $|n_1,\dots,n_\alpha,\dots,n_k>$ is a Fock state constructed with the fermionic creation operator $\left(f_1^\dagger\right)^{n_1}\dots\left(f_\alpha^\dagger\right)^{n_\alpha}\dots\left(f_k^\dagger\right)^{n_k}$ applied on the vacuum state $|0>$. The ξ_α are *Grassmann* variables verifying the anticommutation relations

$$\begin{aligned}
\{\xi_\alpha,\xi_\lambda\}=\xi_\alpha\xi_\lambda+\xi_\lambda\xi_\alpha &= 0 &(3.23)\\
\{\xi_\alpha,\xi_\lambda^*\} &= 0 &(3.24)\\
\xi_\alpha^2=(\xi_\alpha^*)^2 &= 0 &(3.25)
\end{aligned}$$

More properties on the *Grassmann* algebra are given in appendix A .
Applying the annihilation operator f_α on the coherent state $|\xi>$ we obtain

$$\begin{aligned}
f_\alpha|\xi> &= \sum_{k=0}^{\infty}\sum_{\{n_\alpha\}=0}^{1}\xi_1^{n_1}\dots\xi_\alpha^{n_\alpha}\dots\xi_k^{n_k}f_\alpha|n_1,\dots,n_\alpha,\dots,n_k>\\
&= \sum_{k=0}^{\infty}\sum_{\substack{\{n_\lambda\}=0,\\ n_\alpha=1}}^{1}\xi_1^{n_1}\dots\xi_\alpha^{n_\alpha}\dots\xi_k^{n_k}(-1)^{\sum_{j=1}^{\alpha-1}n_j}|n_1,\dots,n_\alpha-1,\dots,n_k>\\
&= \sum_{k=0}^{\infty}\sum_{\{n_\alpha\}=0}^{1}(-1)^{\sum_{j=1}^{\alpha-1}n_j}\xi_1^{n_1}\dots\xi_\alpha^{n_\alpha+1}\dots\xi_k^{n_k}|n_1,\dots,n_\alpha,\dots,n_k>\\
&= \xi_\alpha|\xi> \qquad (3.26)
\end{aligned}$$

Thus ξ_α and $|\xi>$ are the eigenvalue and the eigenvector of the fermionic annihilation operator f_α. Since $f_\alpha^\dagger$ increases the number of particles in any Fock state by one, $|\xi>$ cannot be an eigenvector of $f_\alpha^\dagger$.

Coherent states are equivalently constructed combining the properties of the *Grassmann* variables in exponential series such as

$$|\xi> \;=\; e^{-\sum_\alpha \xi_\alpha f^\dagger_\alpha}|0> = \prod_\alpha (1-\xi_\alpha f^\dagger_\alpha)|0> \tag{3.27}$$

where $|0>$ is the vacuum state of the fermionic Fock space. Similary the *bras* of the coherent states $|\xi>$ verify

$$< \xi| \;=\; <0|e^{-\sum_\alpha f_\alpha \xi^*_\alpha} = <0|e^{\sum_\alpha \xi^*_\alpha f_\alpha} \tag{3.28}$$

$$< \xi|f^\dagger_\alpha \;=\; <\xi|\xi^*_\alpha \tag{3.29}$$

Useful properties can be extracted from these basic equalities.

3.3.2 Properties of the coherent states

In this subsection we review some properties of the coherent states $|\xi>$ which will be used later in the construction of path integrals. The first one is the closure relation in the fermionic Fock space and the second is the trace of a fermionized operator $\mathcal{O}$.

We recall some main points concerning the closure relation of coherent states which reads

$$\int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha}|\xi><\xi| = \mathbb{1} \tag{3.30}$$

A detailed demonstration can be found in the book of Negele and Orland [61]. To proceed, we define the operator $\mathcal{A}$ as being the left hand side of equation (3.30). Following Negele and Orland, the first step in the demonstration of the equality (3.30) is to show that the operator $\mathcal{A}$ is proportional to the unit operator $\mathbb{1}$, the second step to show that the proportionality factor κ is equal to one.

Using the expression (3.27) and the definition of the derivation operator given in appendix A the commutation relation of f_β and the operator $|\xi><\xi|$ is given by

$$\begin{aligned}
[f_\beta, |\xi><\xi|] &= f_\beta|\xi><\xi| - |\xi><\xi|f_\beta \\
&= \xi_\beta|\xi><\xi| - |\xi>\frac{\partial}{\partial \xi^*_\beta}<\xi| \\
&= \left[\xi_\beta - \frac{\partial}{\partial \xi^*_\beta}\right]|\xi><\xi|
\end{aligned} \tag{3.31}$$

Using the properties of the integration operator (see appendix A) the commutation relation of the operator $\mathcal{A}$ and the annihilation operator f_β is equal to zero by virtue of the *Grassmann* algebra

$$
\begin{aligned}
< n_\gamma | \left[f_\beta , \mathcal{A} \right] | n_\lambda > &= < n_\gamma | \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \left[\xi_\beta - \frac{\partial}{\partial \xi^*_\beta} \right] | \xi >< \xi | | n_\lambda > \\
&= \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \left[\xi_\beta - \frac{\partial}{\partial \xi^*_\beta} \right] \xi_\gamma \xi^*_\lambda \\
&= \int \prod_{\alpha = \{\beta,\gamma,\lambda\}} \left(d\xi^*_\alpha d\xi_\alpha \left(1 - \xi^*_\alpha \xi_\alpha\right)\right) \left[\xi_\beta \xi_\gamma \xi^*_\lambda + \xi_\gamma \delta_{\beta\lambda} \right] \\
&= 0
\end{aligned} \tag{3.32}
$$

This equality can also be proven with the use of the creation operator $f^\dagger_\beta$. Therefore the operator $\mathcal{A}$ commutes with any operator composed of operators f_α and $f^\dagger_\alpha$. Since the *Schur* lemma stipulates that if an operator commutes with any operator then it must be proportional to the unit operator. $\mathcal{A}$ must be proportional to the unit operator $\mathbb{1}$, $\mathcal{A} = \kappa \mathbb{1}$.
The matrix element of $\mathcal{A}$ between two vacuum states is given by

$$
\begin{aligned}
< 0 | \mathcal{A} | 0 > &= < 0 | \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} | \xi >< \xi | | 0 > \\
&= \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \\
&= \prod_\alpha 1 = < 0 | \kappa \mathbb{1} | 0 > = \kappa
\end{aligned} \tag{3.33}
$$

Hence $\kappa = 1$.

The closure relation is very useful in order to define the trace of a fermionic operator $\mathcal{O}$. Using the previously defined expression of the trace in the fermion Fock space given in Negele and Orland's book [61]

$$
\begin{aligned}
Tr\left[\mathcal{O}\right] &= \sum_{\{n_{i,\sigma} \in [0,1]\}} \left(\bigotimes_i < n_{i,\uparrow}, n_{i,\downarrow} | \right) \mathcal{O} \left(\bigotimes_i | n_{i,\uparrow}, n_{i,\downarrow} > \right) \\
&\equiv \sum_n < n | \mathcal{O} | n >
\end{aligned} \tag{3.34}
$$

and inserting relation (3.30) into the trace of the operator $\mathcal{O}$, we obtain :

$$
\begin{aligned}
Tr\left[\mathcal{O}\right] &= \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \sum_n < n | \xi >< \xi | \mathcal{O} | n > \\
&= \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} < -\xi | \mathcal{O} \sum_n | n >< n | | \xi > \\
Tr\left[\mathcal{O}\right] &= \int \prod_\alpha d\xi^*_\alpha d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} < -\xi | \mathcal{O} | \xi >
\end{aligned} \tag{3.35}
$$

where $< -\xi|\mathcal{O}\left(\{f_\alpha\},\{f_\alpha^\dagger\}\right)|\xi >= e^{-\sum_\alpha \xi_\alpha^*\xi_\alpha}\mathcal{O}\left(\{-\xi_\alpha\},\{\xi_\alpha^*\}\right)$.

These results complete the tools which enable the construction of the path integral (3.21).

3.3.3 Partition function of many-body systems

In this subsection we construct the partition function of a many-body Hamiltonian in a path integral formulation and we follow the prescription given in [61]. We start with the grand-canonical partition function of a general fermionic Hamiltonian $\tilde{H}$ in Fock space

$$\mathcal{Z} = Tr\left[e^{-\beta\left(\tilde{H}-\mu\tilde{N}\right)}\right] \tag{3.36}$$

Using the Lie-Trotter relation $\lim_{M\to\infty}\left(e^{-\mathcal{A}/M}e^{-\mathcal{B}/M}\right)^M = e^{-(\mathcal{A}+\mathcal{B})}$ equation (3.36) can be reexpressed as $\mathcal{Z} = \lim_{M\to\infty} Tr\left[\left(e^{-\varepsilon\left(\tilde{H}-\mu\tilde{N}\right)}\right)^M\right]$, with $\varepsilon = \beta/M$. Inserting the closure relation (3.30) between each operator $e^{-\varepsilon\left(\tilde{H}-\mu\tilde{N}\right)}$ and using the expression of the trace over coherent states equation (3.35), the partition function takes the form

$$\begin{aligned}
\mathcal{Z} &= \lim_{M\to\infty}\int\prod_{k=1}^{M}\prod_{\alpha} d\xi_{k,\alpha}^* d\xi_{k,\alpha} < -\xi_M|e^{-\varepsilon\left(\tilde{H}-\mu\tilde{N}\right)}|\xi_{M-1}>< \xi_{M-1}|\dots|\xi_k>< \xi_k| \\
&\quad \dots|\xi_2>< \xi_2|e^{-\varepsilon\left(\tilde{H}-\mu\tilde{N}\right)}|\xi_1> \\
&= \lim_{M\to\infty}\int\prod_{k=1}^{M}\prod_{\alpha} d\xi_{k,\alpha}^* d\xi_{k,\alpha} e^{-S(\xi^*,\xi)} \\
-S(\xi^*,\xi) &= \varepsilon\sum_{k=2}^{M}\left[\sum_\alpha \xi_{\alpha,k}^*\{\frac{\xi_{\alpha,k}-\xi_{\alpha,k-1}}{\varepsilon} - \mu\xi_{\alpha,k-1}\} + H(\xi_{\alpha,k}^*,\xi_{\alpha,k-1})\right] \\
&+ \varepsilon\left[\sum_\alpha \xi_{\alpha,1}^*\{\frac{\xi_{\alpha,1}+\xi_{\alpha,M}}{\varepsilon} + \mu\xi_{\alpha,M}\} + H(\xi_{\alpha,1}^*,-\xi_{\alpha,M})\right]
\end{aligned} \tag{3.37}$$

where α refers to the particle position and its spin, and k to the slice in which the term $e^{-\varepsilon\left(\tilde{H}-\mu\tilde{N}\right)}$ appear in the Lie-Trotter formula. It is convenient to introduce the continuum notation $\xi_\alpha(\tau)$ to represent the set $\{\xi_{\alpha,1},\dots,\xi_{\alpha,k},\dots,\xi_{\alpha,M}\}$ and in the limit of $M\to\infty$ to define

$$\xi_{\alpha,k}^*\frac{(\xi_{\alpha,k}-\xi_{\alpha,k-1})}{\epsilon} \equiv \xi_\alpha^*(\tau)\frac{\partial}{\partial\tau}\xi_\alpha(\tau) \tag{3.38}$$

The partition function $\mathcal{Z}$ of the many-body Hamiltonian $\tilde{H}$ with a chemical potential μ takes the functional integral form

$$
\mathcal{Z} = \int_{\xi_\alpha(\beta)=-\xi_\alpha(0)} \mathcal{D}\xi e^{-\int_0^\beta d\tau \{\sum_\alpha \xi_\alpha^*(\tau)(\partial_\tau - \mu)\xi_\alpha(\tau) + H(\xi_\alpha^*(\tau),\xi_\alpha(\tau))\}} \tag{3.39}
$$

where $\mathcal{D}\xi \equiv \lim_{M\to\infty} \prod_{k=1}^{M} \prod_\alpha d\xi_{k,\alpha}^* d\xi_{k,\alpha}$. Expression (3.39) is applicable for general fermionic Hamiltonian operators, in particular for the description of spin systems in terms of path integrals. In the next subsection we introduce a Fourier transform with respect to the imaginary time τ. This leads to Matsubara frequencies which are shifted by the presence of the imaginary chemical potential μ.

3.3.4 Modified Matsubara frequencies

Here we show how the Matsubara frequencies are modified by the introduction of an imaginary chemical potential in the partition function of an spin-1/2 Heisenberg model. As we already saw above Popov and Fedotov introduced the imaginary chemical potential $\mu = i\frac{\pi}{2\beta}$ in order to remove the *unphysical* states of the Fock space as explained in section 3.2 and in [66]. Introducing this chemical potential in the term $\int_0^\beta d\tau \{\sum_\alpha \xi_\alpha^*(\tau)(\partial_\tau - \mu)\xi_\alpha(\tau)$ of equation (3.39) the Fourier transform of $\xi_\alpha(\tau)$ reads

$$
\xi_\alpha(\tau) = \sum_{\omega_F} \xi_\alpha(\omega_F) e^{i\omega_F \tau} \tag{3.40}
$$

and its reverse

$$
\xi_\alpha(\omega_F) = \frac{1}{\beta} \int_0^\beta d\tau \xi_\alpha(\tau) e^{-i\omega_F \tau} \tag{3.41}
$$

Here $\omega_F = \frac{2\pi}{\beta}(n + 1/2)$ with $n \in \mathbb{Z}$ are the well known fermionic Matsubara frequencies. This leads to

$$
\int_0^\beta d\tau \sum_\alpha \xi_\alpha^*(\tau)(\partial_\tau - \mu)\xi_\alpha(\tau) = \sum_{\omega_F} \sum_\alpha \xi_\alpha^*(\omega_F) i(\omega_F - \frac{\pi}{2\beta})\xi_\alpha(\omega_F) \tag{3.42}
$$

Since the chemical potential is imaginary we see that we can redefine the fermionic Matsubara frequencies by the change of variable

$$
\tilde{\omega}_F = \omega_F - \frac{\pi}{2\beta} = \frac{2\pi}{\beta}(n + 1/4) \tag{3.43}
$$

Redefining the Fourier transform of $\xi_\alpha(\tau)$ as

$$\xi_\alpha(\tau) = \sum_{\tilde{\omega}_F} \xi_\alpha(\tilde{\omega}_F) e^{i\tilde{\omega}_F \tau} \tag{3.44}$$

and shifting the partial derivative over τ, $\frac{\partial}{\partial\tau} - \mu \rightarrow \frac{\partial}{\partial\tau}$, the partition function takes the form

$$\begin{aligned} \mathcal{Z} &= \int_{\xi_\gamma(\beta)=i\xi_\gamma(0)} \mathcal{D}\xi e^{-S(\xi^*,\xi)} \\ S(\xi^*_\alpha(\tau), \xi_\alpha(\tau)) &= \sum_{\alpha=(\vec{r}_i,\sigma)} \left(\xi^*_\alpha(\tau) \frac{\partial}{\partial\tau} \xi_\alpha(\tau) \right) + H(\{\xi^*_\alpha(\tau)\}, \{\xi_\alpha(\tau)\}) \end{aligned} \tag{3.45}$$

The partition function itself does not change much by the introduction of the imaginary chemical potential $\mu = i\frac{\pi}{2\beta}$. However the antiperiodic integration condition $\xi_\gamma(\beta) = -\xi_\gamma(0)$ needs to be changed into $\xi_\gamma(\beta) = i\xi_\gamma(0)$ by modification of the Matsubara frequencies. In the following chapters, we will show how these modified fermionic Matsubara frequencies $\tilde{\omega}_F = \frac{2\pi}{\beta}(n + 1/4)$ change the behaviour of the physical properties of spin-1/2 systems.

Chapter 4

Mean-field and fluctuation contributions to the magnetic properties of Heisenberg models

Contents

This chapter intends to present and discuss applications of the mean-field and loop expansion to the determination of physical properties of antiferromagnetic Heisenberg-type systems in spatial dimension D using the PFP. This original point of the present work was published in [21].

Recent work on quantum spin systems discusses the possible existence of spin liquid states and in two space dimensions the competition or phase transition between spin liquid states and an antiferromagnetic Néel state which is naturally expected to describe Heisenberg type systems [28, 57, 74, 75]. It is also known that undoped superconducting systems show an antiferromagnetic phase [50].

In the following we focus our attention on a mean-field Néel phase description of quantum spin systems described by Heisenberg models. More precisely we present below a detailed study of the magnetization and the parallel magnetic susceptibility of Heisenberg antiferromagnetic spin-1/2 systems on D-dimensional lattices at finite temperature. The aim of the work is the study of the physical pertinence of the Néel state ansatz, using the PFP, as a mean-field approximation in the temperature interval $0 < T < T_c$ where T_c is the critical temperature [21]. In order to get a precise answer to this point we work out the quantum and thermal fluctuation contributions beyond the mean-field approximation under the constraint of *strict* single site-occupancy [9, 21, 22, 42, 66] which allows to avoid a Lagrange multiplier approximation [7]. The results are also extended to anisotropic XXZ systems and compared to those obtained in the framework of the spin-wave theory.

4.1 Nearest-Neighbour Heisenberg model

In order to focus on the essential properties of a Néel state mean-field we consider a Heisenberg model which present a bipartite spin lattice. A bipartite lattice can be split into two disjoint sublattices A and B, where J_{ij} connects only $i \in A$ to $j \in B$ as defined in [8]. The simplest isotropic Heisenberg model showing a bipartite lattice reads

$$H = -\frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i.\vec{S}_j + \sum_i \vec{B}_i.\vec{S}_i \tag{4.1}$$

with

$$J_{ij} = J \sum_{\vec{\eta}\in\{\vec{a}_1,\ldots,\vec{a}_D\}} \delta\left(\vec{r}_i - \vec{r}_j \pm \vec{\eta}\right) \tag{4.2}$$

where J is the negative antiferromagnet exchange coupling working between nearest neighbour sites i and j separated by the lattice vector $\vec{\eta} \in \{\vec{a}_1, \ldots, \vec{a}_D\}$ on a D-dimensional lattice. Keeping the static external magnetic field always fixed in the Oz direction the Hamiltonian reads

$$H = -J \sum_{<i,j>} \vec{S}_i.\vec{S}_j + \sum_i B_i.S_i^z \tag{4.3}$$

where the sum $\sum\limits_{<i,j>}$ runs over the nearest neighbour site $< i, j >$ at position $\vec{r}_i \in A$ and $\vec{r}_j \in B$.

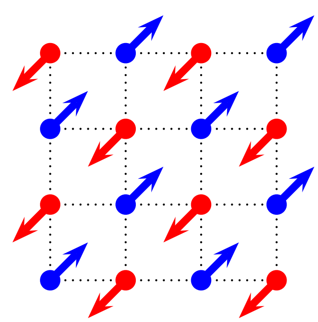


Figure 4.1: A two dimensional bipartite lattice system in a Néel state.

Figure 4.1 is a two-dimensional representation of a bipartite lattice. The spin sublattice A and B are represented by blue and red arrows, dotted lines materialize the exchange interaction $J < 0$ between spins (the blue and red arrows).

4.2 Spin-wave theory

A few years ago Coldea *et al.* [17] measured the magnetic excitations of the square-lattice spin-1/2 antiferromgnet and high-T_c parent compound La_2CuO_4. They showed that the inclusion of some interactions beyond the nearest-neighbour Heisenberg term (4.2) leads to a good description of the dispersion relation observed by high-resolution inelastic neutron scattering in the framework of spin-wave theory.

A modified spin-wave theory developed by Takahashi [77] led to the Auerbach and Arovas equations [7] which were obtained by Schwinger-boson formulation.

In this section we calculate the sublattice magnetization as well as the magnetic susceptibility in the framework of spin-wave theory applied on the nearest neighbour antiferromagnet Heisenberg model (4.3). Later these results will be compared to those obtained using the Popov-Fedotov procedure with the Hamiltonian (4.3).

4.2.1 The Holstein-Primakoff approach

In a broken symmetry phase such as the Néel state at least one spin component shows a non-zero expectation value. For small temperatures the fluctuations about this expectation value can be studied by means of the Holstein and Primakoff (H-P) spin-deviation creation and annihilation boson operators a_i and $a_i^\dagger$.

Since the external magnetic field is applied in the Oz direction the non-zero spin component is S^z. Following H-P we express the spin operators in the form [36]

$$\begin{aligned} S_i^+ &= \sqrt{2S - n_i^a}\, a_i \\ S_i^- &= a_i^\dagger \sqrt{2S - n_i^a} \\ S_i^z &= S - n_i^a \end{aligned} \tag{4.4}$$

where $n_i^a = a_i^\dagger a_i = S - S_i^z$ is the so called spin-deviation operator, a_i and $a_i^\dagger$ are boson operators. Here S is defined from the relation $\vec{S}^2 = S\,(S+1)$ of the quantum spin vector $\vec{S}$. For small temperatures and/or for large-S the expectation value of the spin-deviation operator $< n_i^a >$ is small compared to $2S$ and leads to

$$\sqrt{2S - n_i^a} = (2S)\left(1 - \frac{n_i^a}{4S} - \frac{(n_i^a)^2}{32S^2} + \dots\right) \tag{4.5}$$

Since the Hamiltonian (4.3) shows a bipartite structure on the lattice the spin expectation values are of opposite sign from sublattice A to sublattice B as depicted in figure 4.1. We can define two type of spin operators depending to which sublattice (A or B) they belong. Introducing (4.5) into (4.4) and neglecting all terms n_i^a/S the spin components for sublattice A read

$$\begin{aligned} S_{A,i}^+ &= \sqrt{2S}\, a_i \\ S_{A,i}^- &= a_i^\dagger \sqrt{2S} \\ S_{A,i}^z &= S - n_i^a \end{aligned} \tag{4.6}$$

and for the sublattice B

$$\begin{aligned} S^+_{B,j} &= \sqrt{2S}\,a^\dagger_j \\ S^-_{B,j} &= a_j\,\sqrt{2S} \\ S^z_{B,j} &= -S + n^a_j \end{aligned} \tag{4.7}$$

Following Igarashi [38], Kubo [46], Oguchi [63] and Takahashi [77] the use of (4.6) and (4.7) in (4.3) leads to

$$\begin{aligned} H_{SW} &= |J|\sum_{i\in A}\sum_{\substack{j\in B,\\ \vec{r}_j=\vec{r}_i+\vec{\eta}}}\left(S^z_{A,i}S^z_{B,j}+\frac{1}{2}\left[S^+_{A,i}S^-_{B,j}+S^-_{A,i}S^-_{B,j}\right]\right) \\ &+ \sum_{i\in A}B_iS^z_{A,i}+\sum_{j\in B}B_jS^z_{B,j} \\ &= -\frac{\mathcal{N}}{2}z|J|S^2+z|J|S\left[\sum_{i\in A}(1-\mathcal{B}_i)\,a^\dagger_ia_i+\sum_{j\in B}(1+\mathcal{B}_j)\,a^\dagger_ja_j\right] \\ &\quad +|J|S\sum_{i\in A}\sum_{j\in B}\left(a_ia_j+a^\dagger_ia^\dagger_j\right) \end{aligned} \tag{4.8}$$

where $\mathcal{N}$ is the total number of spin-S in the system and $z = 2D$ is the coordination of a spin in a D-dimensional hypercubical lattice. The magnetic field $\mathcal{B}_i$ is redefined as $\mathcal{B}_i = \frac{B_i}{z|J|S}$. Since we admit that the expectation value of the spin-derivation operator $< n^a >$ is small only quadratic terms in the boson operator a appear in the Hamiltonian (4.8) which amounts to neglect the interaction between spin-waves.

The spin-wave partition function $\mathcal{Z}_{\mathcal{SW}}$ at finite temperature reads

$$\mathcal{Z}_{\mathcal{SW}} = Tr\left[e^{\beta H_{SW}(\{B_i\})}\right] \tag{4.9}$$

Magnetization and susceptibility of the spin system will be extracted from (4.9) taking derivatives with respect to the magnetic field B_i.

4.2.2 Néel Spin-wave magnetization

In order to derive the sublattice magnetization $m_{A(B)}$ from the spin-wave free energy $\mathcal{F}_{SW} = -\frac{1}{\beta}\ln\mathcal{Z}_{SW}$ we set $B_i = B$ if i belongs to sublattice A sites and $B_i = -B$ if it belongs to sublattice B. Taking the derivative with respect to B in (4.9) we obtain

$$\begin{aligned} m_A &= \frac{1}{\mathcal{N}}\left(\sum_{i\in A} < S^z_{A,i} >_{SW} -\sum_{j\in B} < S^z_{B,j} >_{SW}\right) \\ &= -m_B = -\frac{1}{\mathcal{N}\beta}\frac{\partial}{\partial B}\ln\mathcal{Z}_{SW}\Big|_{B=0} = \frac{1}{\mathcal{N}}\frac{\partial}{\partial B}\mathcal{F}_{SW}\Big|_{B=0} \end{aligned} \tag{4.10}$$

Define the Fourier transform of the boson operator a

$$a_i = \frac{1}{\sqrt{\mathcal{N}_A/2}} \sum_{\vec{k}\in SBZ} b^{(1)}_{\vec{k}} e^{i\vec{k}.\vec{r}_i} \tag{4.11}$$

$$a_j = \frac{1}{\sqrt{\mathcal{N}_B/2}} \sum_{\vec{k}\in SBZ} b^{(2)}_{\vec{k}} e^{i\vec{k}.\vec{r}_j} \tag{4.12}$$

where SBZ is the Spin Brillouin Zone which is shown in Figure 4.2 (shaded area) inside the lattice Brillouin Zone of a two dimensional bipartite spin system (large square). More details on the construction of the Spin Brillouin Zone are given in appendix B.

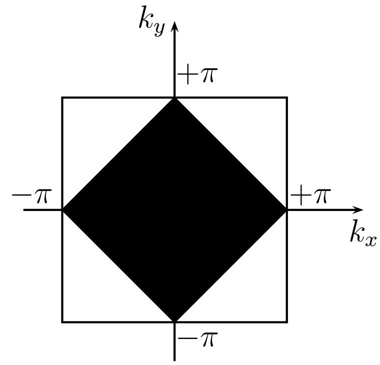


Figure 4.2: Two dimensional Spin Brillouin Zone (shaded area)

Fourier transforming (4.8) with the definitions (4.11) and (4.12) the Hamiltonian goes over to

$$\begin{aligned} H_{SW} &= -\frac{\mathcal{N}}{2} z|J|S^2 + \mathcal{N} z|J|\mathcal{B}S^2 + z|J|S \sum_{\vec{k}\in SBZ} \left[(1-\mathcal{B})\, b^{(1)\dagger}_{\vec{k}} b^{(1)}_{\vec{k}} + (1-\mathcal{B})\, b^{(2)\dagger}_{\vec{k}} b^{(2)}_{\vec{k}} \right] \\ &\quad + z|J|S \sum_{\vec{k}\in SBZ} \gamma_{\vec{k}} \left[b^{(1)}_{\vec{k}} b^{(2)}_{-\vec{k}} + b^{(1)\dagger}_{\vec{k}} b^{(2)\dagger}_{-\vec{k}} \right] \end{aligned} \tag{4.13}$$

where $\gamma_{\vec{k}}$ is the Fourier transform of $\sum_{\vec{\eta}} \delta\left(\vec{r}_i - \vec{r}_j + \vec{\eta}\right)$ and $\vec{\eta}$ was defined in equation (4.2), section 4.1. γ is related to $\vec{\eta}$ by

$$\gamma_{\vec{k}} = \frac{1}{z} \sum_{\vec{\eta}\in\{\pm\vec{a}_1,\ldots,\pm\vec{a}_D\}} e^{i\vec{k}.\vec{\eta}} \tag{4.14}$$

Notice that the coordination z is simply related to the lattice vectors by $z = \sum_{\vec{\eta}\in\{\pm\vec{a}_1,\ldots,\pm\vec{a}_D\}} 1$.

The Hamiltonian (4.13) can be diagonalized by means of a Bogoliubov transformation applied to the boson operators $b, b^\dagger$ [14, 15]

$$\begin{pmatrix} b^{(1)}_{\vec{k}} \\ b^{(2)\dagger}_{-\vec{k}} \end{pmatrix} = \begin{bmatrix} u_{\vec{k}} & v_{\vec{k}} \\ v_{\vec{k}} & u_{\vec{k}} \end{bmatrix} \begin{pmatrix} \beta_{(+),\vec{k}} \\ \beta^\dagger_{(-),-\vec{k}} \end{pmatrix} \tag{4.15}$$

where $u_{\vec{k}}$ and $v_{\vec{k}}$ are real coefficients verifying $u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1$ as a consequence of the commutation relations obeyed by the boson operators $\beta_{(+),\vec{k}}$ and $\beta_{(-),\vec{k}}$. We set $u_{\vec{k}} = \cosh\theta_{\vec{k}}$ and $v_{\vec{k}} = \sinh\theta_{\vec{k}}$. Using (4.15) leads to the diagonalized Hamiltonian (4.13)

$$
\begin{aligned}
H_{SW} &= -\frac{\mathcal{N}}{2} z|J|S^2 + z|J|\mathcal{N}\mathcal{B}S^2 - \frac{\mathcal{N}}{2} z|J|S\,(1-\mathcal{B}) \\
&\quad + \sum_{\vec{k}\in SBZ} \omega_{\vec{k}} \left(\beta^{\dagger}_{(+),\vec{k}}\beta_{(+),\vec{k}} + \beta^{\dagger}_{(-),\vec{k}}\beta_{(-),\vec{k}} + 1\right) \qquad (4.16)
\end{aligned}
$$

with

$$
\begin{aligned}
\tanh 2\theta_{\vec{k}} &= -\frac{\gamma_{\vec{k}}}{(1-\mathcal{B})} \qquad (4.17) \\
\omega_{\vec{k}} &= z|J|S\sqrt{(1-\mathcal{B}) - \gamma_{\vec{k}}^2} \qquad (4.18)
\end{aligned}
$$

Here $\omega_{\vec{k}}$ is the spin-wave spectrum and $\beta^{\dagger}_{(\pm),\vec{k}}\beta_{(\pm),\vec{k}}$ is the number operator of *magnons* occupying the energy "level" $\omega_{\vec{k}}$. In the absence of the magnetic field $\mathcal{B}$ and for $\vec{k}$ close to $\vec{Q} = 0$ or $\vec{\pi}$ ($\vec{\pi} = (\pi, \ldots, \pi)$) the dispersion relation shows a relativistic spectrum $\omega_{\vec{k}} \sim c|\vec{k} - \vec{Q}|$ where c is the spin-wave velocity for a D-dimensional hypercubical lattice, $c = \sqrt{D}|J|S$.

The sublattice magnetization $m_A = -m_B$ is derived from the spin-wave free energy $\mathcal{F}_{SW} = -\frac{1}{\beta}\ln Tr\left[e^{-\beta H_{SW}}\right]$ and reads

$$
\begin{aligned}
m_A &= 1 - \frac{1}{\mathcal{N}} \sum_{\vec{k}\in SBZ} \frac{1}{\tanh\frac{\beta}{2}\omega_{\vec{k}}} . \frac{1}{\sqrt{1-\gamma_{\vec{k}}^2}} \\
&= 1 - \frac{1}{\mathcal{N}} \sum_{\vec{k}\in BZ} \left(n_{\vec{k}} + \frac{1}{2}\right) . \frac{1}{\sqrt{1-\gamma_{\vec{k}}}} \qquad (4.19)
\end{aligned}
$$

$n_{\vec{k}} = \frac{1}{e^{\beta\omega_{\vec{k}}}-1}$ is the boson occupation number. Notice that in the second equation of m_A the sum runs over the whole Brillouin Zone. Later the magnetization (4.19) will be used as a reference for comparaison with the magnetization obtained by means of our method using the PFP.

4.2.3 Néel Spin-wave susceptibility

With a uniform magnetic field $B_i = B$ applied on the spin system the spin-wave susceptibility is obtained from the free energy by

$$
\chi_{\parallel} = -\frac{\partial^2 \mathcal{F}_{SW}}{\partial B^2}\bigg|_{B=0} \qquad (4.20)
$$

where $\mathcal{F}_{SW} = -\frac{1}{\beta}\ln \mathcal{Z}_{SW} = -\frac{1}{\beta}\ln Tr\left[e^{-\beta H_{SW}}\right]$ and the spin-wave Hamiltonian H_{SW}

$$
\begin{aligned}
H_{SW} &= -\frac{\mathcal{N}}{2} z|J|S^2 + z|J|S\left[\sum_{i\in A}(1-\mathcal{B})\,a_i^\dagger a_i + \sum_{j\in B}(1+\mathcal{B})\,a_j^\dagger a_j\right] \\
&\quad +|J|S\sum_{i\in A}\sum_{j\in B}\left(a_i a_j + a_i^\dagger a_j^\dagger\right) \qquad (4.21)
\end{aligned}
$$

A Bogoliubov transformation leads to the diagonalized spin-wave Hamiltonian

$$
\begin{aligned}
H_{SW} &= -\frac{N}{2} z|J|S^2 + z|J|S\sum_{\vec{k}\in SBZ}\Big[\omega_{\vec{k}} + \left(\omega_{\vec{k}}+\mathcal{B}\right)\beta^\dagger_{(+),\vec{k}}\beta_{(+),\vec{k}} \\
&\quad + \left(\omega_{\vec{k}}-\mathcal{B}\right)\beta^\dagger_{(-),\vec{k}}\beta_{(-),\vec{k}}\Big] \qquad (4.22) \\
\tanh\left(2\theta_{\vec{k}}\right) &= -\gamma_{\vec{k}} \qquad (4.23) \\
\omega_{\vec{k}} &= z|J|S\sqrt{1-\gamma^2_{\vec{k}}} \qquad (4.24)
\end{aligned}
$$

$\mathcal{B} = B/z|J|S$. The free energy is then given by

$$
\begin{aligned}
\mathcal{F}_{SW} &= -\frac{1}{\beta}\ln \mathcal{Z}_{SW} \\
&= -\frac{1}{\beta}\sum_{\vec{k}\in SBZ}\left[-\beta\omega_{\vec{k}} - \ln\left[1-e^{-\beta\left(\omega_{\vec{k}}+\mathcal{B}\right)}\right]\left[1-e^{-\beta\left(\omega_{\vec{k}}-\mathcal{B}\right)}\right]\right] \qquad (4.25)
\end{aligned}
$$

Finally the spin-wave susceptibility reads

$$
\begin{aligned}
\chi_\parallel &= -\left.\frac{\partial^2\mathcal{F}_{SW}}{\partial B^2}\right|_{B=0} \\
&= 2\beta\sum_{\vec{k}\in SBZ} n_{\vec{k}}\left(n_{\vec{k}}+1\right) \qquad (4.26)
\end{aligned}
$$

where $n_{\vec{k}} = \frac{1}{e^{\beta\omega_{\vec{k}}}-1}$ is the boson occupation number of the magnons.

4.3 Effective action

After this review on spin-wave theory we return to the study of the Heisenberg model by functional integrals. The aim of this work is to extract the magnetization and the spin susceptibility from the path integral formulation (see section 3, equation (3.45)) for the Hamiltonian (4.3) of a bipartite spin system in a Néel state. As we shall see later the analytic development of the effective action necessitates some approximations. In order to be able to appreciate the pertinence of these approximations, that is the Néel mean-field with the one-loop corrections for example, we define a “Ginzburg-Landau parameter” which evaluates the relative importance of the quantum and thermal fluctuations on the mean-field Néel state. We compare the magnetization and the susceptibility worked out from functional integral formulation with those obtained from the spin-wave theory for the Hamiltonian (4.3).

4.3.1 The Hubbard-Stratonovich transform

As was shown in chapter 3 the Hamiltonian (4.3) can be expressed in terms of creation and annihilation fermion operators $f^{\dagger}$ and f by replacing the spin operator $\vec{S}_i$ by (3.2). Performing this transformation and injecting the resulting fermionic Hamiltonian (4.3) into the path integral (3.45) we see that the term $\vec{S}_i.\vec{S}_j$ in the exponent leads to a quartic expression in the *Grassmann* variables

$$\begin{aligned} S\left(\xi^{*},\xi\right) &= \sum_{\alpha=\vec{r}_i,\sigma}\left(\xi_{\alpha}^{\dagger}\left(\tau\right)\frac{\partial}{\partial\tau}\xi_{\alpha}\left(\tau\right)\right)+H\left(\xi^{*},\xi\right) \\ H\left(\xi^{*},\xi\right) &= \sum_{i}B_i.\frac{1}{2}\left(\xi_{i,\uparrow}^{*}(\tau)\xi_{i,\uparrow}(\tau)-\xi_{i,\downarrow}^{*}(\tau)\xi_{i,\downarrow}(\tau)\right) \\ &- \sum_{<i,j>}J\left(\xi_{i,\sigma_1}^{*}(\tau)\vec{\sigma}_{\sigma_1\sigma_2}\xi_{i,\sigma_2}(\tau)\right).\left(\xi_{j,\sigma_3}^{*}(\tau)\vec{\sigma}_{\sigma_3\sigma_4}\xi_{j,\sigma_4}(\tau)\right) \end{aligned} \tag{4.27}$$

where repeated indices mean summations over them. Recall that $\vec{\sigma}$ are the $SU(2)$ Pauli matrices defined in 3.2. Since integration over the *Grassmann* variables of the path integral (3.45) is not possible as it stands we have to reduce the action (4.27) to a quadratic expression by means of a Hubbard-Stratonovich (HS) transformation [37, 76]. We define the Hubbard-Stratonovich auxiliary field action S_0 as

$$S_0\left[\varphi^{'}(\tau)\right]=\frac{1}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\vec{\varphi^{'}}_i(\tau).\vec{\varphi^{'}}_j(\tau) \tag{4.28}$$

where $\left(J^{-1}\right)_{ij}$ is the inverse of the coupling matrix J_{ij} and $\vec{\varphi}$ is the Hubbard-Stratonovich auxiliary field. The matrix $\left(J^{-1}\right)_{ij}$ always exists if one considers periodic bondary conditions on the spin system. Adding the HS action S_0 to the fermionic Hamiltonian $H\left(\xi^{*},\xi\right)$ and performing the change of variable

$$\vec{\varphi^{'}}_i(\tau)=\vec{\varphi}_i(\tau)+\sum_{j}J_{ij}\vec{S}_j(\tau) \tag{4.29}$$

where $\vec{S}_j(\tau)=\xi_{j,\sigma_1}^{*}(\tau)\vec{\sigma}_{\sigma_1\sigma_2}\xi_{j,\sigma_2}(\tau)$ leads to the Hubbard-Stratonovich transformed Hamiltonian which reads

$$S_0\left[\varphi^{'}(\tau)\right]+H\left(\xi^{*},\xi\right)\rightarrow S_0\left[\varphi(\tau)\right]+\sum_{i}\left(\vec{\varphi}_i(\tau)+\vec{B}_i\right).\vec{S}_i(\tau) \tag{4.30}$$

and the partition function

$$\mathcal{Z} = \frac{1}{\mathcal{Z}_0}\int_{\varphi(\beta)=\varphi(0)} \mathcal{D}\vec{\varphi}\int_{\xi_{i\sigma}(\beta)=i\xi_{i\sigma}(0)} \mathcal{D}\xi e^{-\int_0^\beta d\tau S[\varphi,\xi^*,\xi]} \tag{4.31}$$

$$S\left[\varphi,\xi^*,\xi\right] = \sum_{i,\sigma}\xi^*_{i\sigma}(\tau)\frac{\partial}{\partial\tau}\xi_{i\sigma}(\tau) + S_0\left[\varphi(\tau)\right] + \sum_i\left(\vec{\varphi}_i(\tau)+\vec{B}_i\right).\vec{S}_i(\tau) \tag{4.32}$$

Here $\mathcal{Z}_0$ stands for the partition function of the HS auxiliary field and reads

$$\mathcal{Z}_0 = \int_{\varphi(\beta)=\varphi(0)} \mathcal{D}\vec{\varphi}e^{-\int_0^\beta d\tau S_0[\vec{\varphi}(\tau)]} \tag{4.33}$$

and $\mathcal{D}\vec{\varphi} \equiv \lim_{M\to\infty}\prod_{k=1}^{M}\prod_i d\varphi^x_{i,k}d\varphi^y_{i,k}d\varphi^z_{i,k}$ as explained for the *Grassmann* variables in subsection 3.3.3.

4.3.2 Integration over the *Grassmann* variables

The action (4.32) can also be written as

$$S\left[\varphi,\xi^*,\xi\right] = S_0\left[\varphi(\tau)-B\right] + \sum_i\begin{pmatrix}\xi^*_{i,\uparrow}(\tau) & \xi^*_{i,\downarrow}(\tau)\end{pmatrix}M_i(\tau)\begin{pmatrix}\xi_{i,\uparrow}(\tau)\\ \xi_{i,\downarrow}(\tau)\end{pmatrix} \tag{4.34}$$

after the variable shift $\vec{\varphi}_i(\tau)\to\vec{\varphi}_i(\tau)-\vec{B}_i$. The matrix $M_i(\tau)$ contains the factor of the quadratic terms in the *Grassmann* variables

$$M_i(\tau) = \begin{bmatrix}\frac{\partial}{\partial\tau}+\frac{1}{2}\varphi^z_i(\tau) & \frac{1}{2}\varphi^-_i(\tau)\\ \frac{1}{2}\varphi^+_i(\tau) & \frac{\partial}{\partial\tau}-\frac{1}{2}\varphi^z_i(\tau)\end{bmatrix} \tag{4.35}$$

Fourier transforming (4.34) with the definitions of subsection 3.3.4 one gets

$$\begin{aligned}\int_0^\beta d\tau S\left[\varphi,\xi^*,\xi\right] &= \frac{\beta}{2}\sum_{\omega_{B,n}}\sum_{i,j}\left(J^{-1}\right)_{ij}\left[\vec{\varphi}_i(-\omega_{B,n})-\vec{B}_i\right]\left[\vec{\varphi}_j(\omega_{B,n})-\vec{B}_j\right]\\ &+ \beta\sum_i\sum_{\tilde{\omega}_{F,p},\tilde{\omega}_{F,q}}\begin{pmatrix}\xi^*_{i,\uparrow}(\tilde{\omega}_{F,p}) & \xi^*_{i,\downarrow}(\tilde{\omega}_{F,q})\end{pmatrix}M_i(p-q)\begin{pmatrix}\xi_{i,\uparrow}(\tilde{\omega}_{F,q})\\ \xi_{i,\downarrow}(\tilde{\omega}_{F,q})\end{pmatrix}\end{aligned} \tag{4.36}$$

where $\omega_{B,n}\equiv\frac{2\pi}{\beta}n$ are boson Matsubara frequencies since from equation (4.29) the auxiliary field φ needs to be periodic in τ so that $\vec{\varphi}_i(\beta)=\vec{\varphi}_i(0)$. The modified fermionic Matsubara frequencies $\tilde{\omega}_{F,p}=\frac{2\pi}{\beta}(p+1/4)$ are defined in subsection 3.3.4. After the Fourier transform the matrix M_i reads

$$M_i(p-q) = \begin{bmatrix} i\tilde{\omega}_{F,p}\delta_{p,q} + \frac{1}{2}\varphi_i^z(\tilde{\omega}_{F,p} - \tilde{\omega}_{F,q}) & \frac{1}{2}\varphi_i^-(\tilde{\omega}_{F,p} - \tilde{\omega}_{F,q}) \\ \frac{1}{2}\varphi_i^+(\tilde{\omega}_{F,p} - \tilde{\omega}_{F,q}) & i\tilde{\omega}_{F,p}\delta_{p,q} - \frac{1}{2}\varphi_i^z(\tilde{\omega}_{F,p} - \tilde{\omega}_{F,q}) \end{bmatrix} \tag{4.37}$$

Then after integration over the *Grassmann* variables using equation (A.24) one obtains

$$\mathcal{Z} = \frac{1}{\mathcal{Z}_0}\int_{\varphi(\beta)=\varphi(0)} \mathcal{D}\vec{\varphi}e^{-S_{eff}[\vec{\varphi}]} \tag{4.38}$$

where the effective action S_{eff} reads

$$S_{eff} = \int_0^\beta S_0\left[\varphi(\tau) - B\right] - \sum_i \ln\det\beta M_i \tag{4.39}$$

4.4 Mean-field equation and One-loop contributions

The mean-field equations are obtained from $\frac{\delta S_{eff}}{\delta\varphi} = 0$ which is the stationnarity condition in the application of the least action principle. Assuming that the mean-field and fluctuations contributions of the effective action S_{eff} can be identified and separated, the matrix M can be decomposed into a mean-field part G_0^{-1} and a fluctuation contribution M_1 and thus reads

$$M = -G_0^{-1} + M_1 \tag{4.40}$$

where the mean-field matrix G_0^{-1} depend on the choice of the mean-field Hubbard-Stratonovich auxiliary field $\bar{\vec{\varphi}}$ and M_1 is composed of the fluctuations $\vec{\delta\varphi} = \vec{\varphi} - \bar{\vec{\varphi}}$. At first glance it does not seem obvious to choose the mean-field components of the HS auxiliary field $\bar{\vec{\varphi}}$. From (4.29) it is clear that the mean-field of $\vec{\varphi}$ is related to the mean-field of the spins and thus $\bar{\vec{\varphi}}$ should show the same symmetries as the spin mean-field. When the temperature is increased it is expected that thermal fluctuations $\vec{\delta\varphi}$ become more and more important and the auxiliary field $\vec{\varphi}$ may move away from the mean-field $\bar{\vec{\varphi}}$. Considering the temperature limit $T \to 0$ the boson (and also fermion) Matsubara frequencies $\omega_{B,n}$ go to zero for any value of n. Then the relevant mean-field Fourier components of $\bar{\vec{\varphi}}(\omega_{B,n})$ are those for which $\omega_{B,n} = 0$. Fourier transforming M with respect to the imaginary time τ and extracting the mean-field part $\bar{\vec{\varphi}}$ from M one obtains

$$G_{0p,q} = \begin{bmatrix} -\frac{1}{\det G_p}\left[i\omega_{F,p} - \frac{1}{2}\bar{\varphi}_i^z(\omega_{F,p} - \omega_{F,q})\right]\delta_{p,q} & \frac{1}{\det G_p}\frac{1}{2}\bar{\varphi}_i^-(\omega_{F,p} - \omega_{F,q})\delta_{p,q} \\ \frac{1}{\det G_p}\frac{1}{2}\bar{\varphi}_i^+(\omega_{F,p} - \omega_{F,q})\delta_{p,q} & -\frac{1}{\det G_p}\left[i\omega_{F,p} + \frac{1}{2}\bar{\varphi}_i^z(\omega_{F,p} - \omega_{F,q})\right]\delta_{p,q} \end{bmatrix} \tag{4.41}$$

and the fluctuating part $\vec{\delta\varphi}$ are given by

$$M_{1p,q} = \begin{bmatrix} \frac{1}{2}\delta\varphi_i^z(\omega_{F,p}-\omega_{F,q}) & \frac{1}{2}\delta\varphi_i^-(\omega_{F,p}-\omega_{F,q}) \\ \frac{1}{2}\delta\varphi_i^+(\omega_{F,p}-\omega_{F,q}) & -\frac{1}{2}\delta\varphi_i^z(\omega_{F,p}-\omega_{F,q}) \end{bmatrix} \tag{4.42}$$

with $\delta\vec{\varphi}_i(\omega_{F,p}-\omega_{F,q}) = \vec{\varphi}_i(\omega_{F,p}-\omega_{F,q}) - \bar{\vec{\varphi}}_i(\omega_{F,p}-\omega_{F,q})\delta_{p,q}$ and $\det G_p = -\left[\omega_{F,p}^2 + \left(\frac{\bar{\vec{\varphi}}_\alpha(\omega_{F,p}-\omega_{F,q}=0)}{2}\right)^2\right]$. The expression $\ln\det(\beta M)$ in the effective action (4.39) can now be developed into a series

$$\begin{aligned} \ln\det(\beta M) &= \ln\det\beta\left[-G_0^{-1}(1-G_0M_1)\right] \\ &= \ln\det(-\beta G_0^{-1}) + Tr\ \ln(1-G_0M_1) \\ &= \ln\det(-\beta G_0^{-1}) - Tr\{\sum_{n=1}^{\infty}\frac{1}{n}(G_0M_1)^n\} \end{aligned}$$

The first term $\ln\det(-\beta G_0^{-1})$ leads to the expression $\sum_i \ln 2\cosh\frac{\beta}{2}\|\bar{\vec{\varphi}}_i(\omega_B=0)\|$ and the effective action over the auxiliary field $\vec{\varphi}$ reads

$$S_{eff}\left[\vec{\varphi}\right] = \int_0^\beta d\tau S_0\left[\vec{\varphi}(\tau)\right] - \sum_i \ln 2\cosh\frac{\beta}{2}\|\bar{\vec{\varphi}}_i(\omega_B=0)\| + Tr\left[\sum_{n=1}^{\infty}\frac{1}{n}(G_0M_1)^n\right] \tag{4.43}$$

The first term $n=1$ in the sum over n gives the contributions at the first order in the fluctuations $\delta\varphi$, the second one the one-loop correction to the mean-field for $n=2$. It is quadratic in $\delta\varphi$. Hence in a loop expansion beyond the mean-field approximation $\bar{\vec{\varphi}}$ the effective action given by (4.43) is a Taylor series expansion in powers of $\delta\vec{\varphi}$. To second order (one-loop contribution) in the fluctuations $\delta\vec{\varphi}^{\,2}$ of $\vec{\varphi} = \bar{\vec{\varphi}} + \delta\vec{\varphi}$.

$$S_{eff}\left[\vec{\varphi}\right] = S_{eff}\Big|_{[\bar{\vec{\varphi}}]} + \frac{\delta S_{eff}}{\delta\vec{\varphi}}\Big|_{[\bar{\vec{\varphi}}]}\delta\vec{\varphi} + \frac{1}{2}\frac{\delta^2 S_{eff}}{\delta\vec{\varphi}^{\,2}}\Big|_{[\bar{\vec{\varphi}}]}\delta\vec{\varphi}^2 + \mathcal{O}(\delta\vec{\varphi}^{\,3}) \tag{4.44}$$

We now give a more precise definition of our mean-field $\bar{\vec{\varphi}}$. The partition function (4.38) can be worked out by means of a *saddle-point* method in which $\frac{\partial S_{eff}}{\delta\vec{\varphi}}\Big|_{[\bar{\vec{\varphi}}]}\delta\vec{\varphi} = 0$ and leads to the equation

$$\mathcal{Z} = e^{-S_{eff}\Big|_{[\bar{\vec{\varphi}}]}}.\int\mathcal{D}\delta\varphi e^{-\left(\frac{1}{2}\frac{\delta^2 S_{eff}}{\delta\vec{\varphi}^2}\Big|_{[\bar{\vec{\varphi}}]}\delta\vec{\varphi}^2 + \mathcal{O}(\delta\vec{\varphi}^3)\right)} \tag{4.45}$$

where the mean-field solutions verify the self-consistent set of equations

$$\sum_j \left(J^{-1}\right)_{ij}\left[\bar{\vec{\varphi}}_j - \vec{B}_j\right] = \frac{1}{2}\frac{\bar{\vec{\varphi}}_i}{\bar{\varphi}_i}\tanh\left[\frac{\beta\bar{\varphi}_i}{2}\right] \tag{4.46}$$

These equations lead directly to the cancellation of the first order term in $\delta\vec{\varphi}$ as worked out in appendix C.

In the following we consider a Néel mean-field order $\vec{\bar{\varphi}}_i(\tau) = (-1)^{\vec{\pi}.\vec{r}_i}\bar{\varphi}^z\vec{e}_z = \bar{\varphi}_i^z\vec{e}_z$ where $\vec{\pi}$ is the Brillouin spin sublattice vector as defined in section 4.2. A magnetic field aligned along the direction $\vec{e}_z$ is applied to the system. The partition function can be decomposed into a product of three terms

$$\mathcal{Z} = \mathcal{Z}_{MF}.\mathcal{Z}_{zz}.\mathcal{Z}_{+-} \tag{4.47}$$

where $\mathcal{Z}_{MF}$, $\mathcal{Z}_{zz}$ and $\mathcal{Z}_{+-}$ are given by

$$\begin{aligned}
\mathcal{Z}_{MF} &= e^{-S_{eff}\big|_{[\bar{\varphi}]}} && (4.48)\\
\mathcal{Z}_{zz} &= \frac{1}{\mathcal{Z}_0^{zz}}\int \mathcal{D}\delta\varphi^z e^{-\frac{1}{2}\frac{\partial^2 S_{eff}}{\partial{\varphi^z}^2}\big|_{[\bar{\varphi}]}{\delta\varphi^z}^2} && (4.49)\\
\mathcal{Z}_{+-} &= \frac{1}{\mathcal{Z}_0^{+-}}\int \mathcal{D}(\delta\varphi^+,\delta\varphi^-) e^{-\frac{1}{2}\frac{\partial^2 S_{eff}}{\partial\varphi^+\partial\varphi^-}\big|_{[\bar{\varphi}]}\delta\varphi^+.\delta\varphi^-} && (4.50)
\end{aligned}$$

with

$$S_{eff}\Big|_{[\bar{\varphi}]} = \frac{\beta}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\left[(\bar{\varphi}_i^z - B_i^z).(\bar{\varphi}_j^z - B_j^z)\right] - \sum_i \ln 2\cosh\frac{\beta}{2}\|\bar{\varphi}_i^z\| \tag{4.51}$$

The one-loop corrections $(\delta\varphi^z)^2$ and $\delta\varphi^+\delta\varphi^-$ terms are worked out in details in appendix C and read

$$\begin{aligned}
\frac{1}{2}\frac{\delta^2 S_{eff}}{\delta{\varphi^z}^2}\Big|_{[\bar{\varphi}]}{\delta\varphi^z}^2 =& \sum_{\omega_B}\sum_{i,j}\frac{\beta}{2}\Bigg[\left(J^{-1}\right)_{ij}\\
&-\left(\frac{\beta}{4}\tanh'\left(\frac{\beta}{2}\bar{\varphi}_i^z\right)\right)\delta_{ij}\delta(\omega_B=0)\Bigg]\delta\varphi_i^z(-\omega_B)\delta\varphi_j^z(\omega_B)\\
\frac{1}{2}\frac{\partial^2 S_{eff}}{\delta\varphi^+\delta\varphi^-}\Big|_{[\bar{\varphi}]}\delta\varphi^+\delta\varphi^- =& \sum_{\omega_B}\sum_{i,j}\frac{\beta}{2}\left[\frac{1}{2}\left(J^{-1}\right)_{ij} - \left(\frac{1}{2}\frac{\tanh\left(\frac{\beta}{2}\bar{\varphi}_i^z\right)}{\bar{\varphi}_i^z - i\omega_B}\right)\delta_{ij}\right]\delta\varphi_i^+(-\omega_B)\delta\varphi_j^-(\omega_B)\\
&+\sum_{\omega_B}\sum_{i,j}\frac{\beta}{2}\left[\frac{1}{2}\left(J^{-1}\right)_{ij}\right]\delta\varphi_i^+(\omega_B)\delta\varphi_j^-(-\omega_B)
\end{aligned} \tag{4.52}$$

$\mathcal{Z}_{MF}$ is the mean-field contribution, $\mathcal{Z}_{zz}$ and $\mathcal{Z}_{+-}$ are the one-loop contributions respectively for the longitudinal part $\delta\varphi^z$ and the transverse parts of $\vec{\varphi}$, $\delta\varphi^{+-}$, which take account of the fluctuations around the mean-field value $\bar{\varphi}^z$.

The contributions $\mathcal{Z}_{zz}$ and $\mathcal{Z}_{+-}$ are quadratic in the field variables $\delta\varphi^z, \delta\varphi^{+-}$ and can be worked out in the presence of a staggered magnetic field B_i^z. Studies involving a uniform magnetic field acting on antiferromagnet quantum spin systems can also be found in ref.[42].

4.5 Magnetization and susceptibility for D-dimensional systems

4.5.1 Relation between the Hubbard-Stratonovich auxiliary field and the magnetization

We define by $\mathcal{F}_{MF} \equiv -\frac{1}{\beta}\ln \mathcal{Z}_{MF}$ the mean-field free energy where $\mathcal{Z}_{MF}$ is given by equation (4.48). The local fields $\{\vec{\bar{\varphi}}_i\}$ can be related to the local magnetizations $\{\vec{\bar{m}}_i\}$. Using $\vec{\bar{m}}_i = -\frac{\partial \mathcal{F}_{MF}}{\partial \vec{B}_i}$ one gets

$$\begin{aligned} \vec{\bar{m}}_i &= -\frac{\partial \mathcal{F}_{MF}}{\partial \vec{B}_i} = \frac{1}{\beta}\frac{\partial}{\partial \vec{B}_i} S_{eff}\Big|_{[\bar{\varphi}]} \\ &= \sum_j \left(J^{-1}\right)_{ij}\left[\vec{\bar{\varphi}}_j - \vec{B}_j\right] \end{aligned} \tag{4.53}$$

and from the mean-field relation (4.46) one deduces also the relation

$$\vec{\bar{m}}_i = \frac{1}{2}\frac{\vec{\bar{\varphi}}_i}{\bar{\varphi}_i}\tanh\frac{\beta}{2}\bar{\varphi}_i \tag{4.54}$$

where $\bar{\varphi}_i = \|\vec{\bar{\varphi}}_i\|$. Considering the Néel state $\vec{\bar{\varphi}}_i = \bar{\varphi}_i^z \vec{e}_z$ and keeping the external magnetic field $\vec{B}_i$ applied in the direction Oz one gets

$$\bar{\varphi}_j^z = \frac{2}{\beta}\tanh^{-1}2\bar{m}_i \tag{4.55}$$

$$\bar{\varphi}_j^z - B_j = \sum_j J_{i,j}\bar{m}_j \tag{4.56}$$

Combining (4.55) and (4.56) the self-consistent mean-field equation of the magnetization $\bar{m}_i$ is obtained by means of the set of equations

$$\begin{aligned} \frac{2}{\beta}\tanh^{-1}2\bar{m}_i &= B_i + \sum_j J_{i,j}\bar{m}_j \\ \bar{m}_i &= \frac{1}{2}\tanh\left[\frac{\beta}{2}\left(B_i + \sum_j J_{i,j}\bar{m}_j\right)\right] \end{aligned} \tag{4.57}$$

4.5.2 Linear response theory

The magnetization mean-field equation (4.57) can be solved in the linear response theory. If the applied magnetic field is weak enough the mean-field magnetization $\bar{m}_i$ can be developed linearly with respect to the magnetic field

$$\bar{m}_i \;=\; (-1)^{\vec{r}_i.\vec{\pi}}\bar{m} + \Delta m B_i + \mathcal{O}(B^2) \tag{4.58}$$

where $\vec{\pi}$ is the Brillouin vector coming from the existence of the sublattices in the Néel state defined below (4.46), $\vec{r}_i$ the lattice position, $\bar{m}$ the sublattice magnetization and Δm the linear coefficient in the magnetic field B_i. According to the dependence of the magnetic field on the site i of the lattice and by inspection of (4.58) and (4.57) the linear coefficient Δm reads

$$\Delta m = \begin{cases} \Delta\tilde{m}_0 = \frac{\frac{\beta}{4}\left(1-4\bar{m}^2\right)}{1-\frac{\beta}{2}D|J|(1-4\bar{m}^2)} & \text{, when } B_i = (-1)^{\vec{r}_i.\vec{\pi}}B \\ \Delta m_{\chi 0} = \frac{\frac{\beta}{4}\left(1-4\bar{m}^2\right)}{1+\frac{\beta}{2}D|J|(1-4\bar{m}^2)} & \text{, when } B_i = B. \end{cases} \tag{4.59}$$

where $\bar{m}$ is the mean-field sublattice magnetization without external magnetic field which verifies

$$\bar{m} = \frac{1}{2}th\frac{\beta}{2}D|J|\bar{m} \tag{4.60}$$

The solution depends on the dimension D and the coupling constant J of the nearest-neighbour Heisenberg model (4.3). The self-consistent equation (4.60) is easily solved numerically using the Newton method [67]. As can be seen on figure 4.3 the mean-field magnetization saturates at $1/2$ for the temperature $T = 0$ and vanishes at the critical temperature $T_c \equiv D|J|/2$. Depending on the configuration of the magnetic field one can either compute the magnetization with $B_i = (-1)^{\vec{r}_i.\vec{\pi}}B$ or the susceptibility with $B_i = B$ as was previoulsy explained in section 4.2 concerning spin-wave theory.

4.5.3 Néel magnetization with fluctuation corrections : results

Substituting equation (4.58) with the magnetic field configuration $B_i = (-1)^{\vec{r}_i.\vec{\pi}}B$ and relations (4.55),(4.56) into equations (4.48), (4.49) and (4.50) integrating over the HS auxiliary fluctuation field $\delta\vec{\varphi}$ one obtains the free energy $\mathcal{F}$. The derivation of the free energy is given in details in appendix C. The components $\mathcal{F}_{MF}, \mathcal{F}_{zz}$ and $\mathcal{F}_{+-}$ of the free energy for a linear approximation in the magnetic field read

$$\mathcal{F}_{MF} = \mathcal{N}D|J|\left(\bar{m} + \Delta\tilde{m}_0.B\right)^2 - \frac{\mathcal{N}}{\beta}\ln\cosh\left(\frac{\beta}{2}\left[B + 2D|J|(\bar{m} + \Delta\tilde{m}_0.B)\right]\right) \tag{4.61}$$

$$\delta\mathcal{F}_{zz} = \frac{1}{2\beta}\sum_{\vec{k}\in SBZ} \ln\left[1-\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2\left[1-4(\bar{m}+\Delta\tilde{m}_0.B)^2\right]^2\right] \tag{4.62}$$

$$\begin{aligned}\delta\mathcal{F}_{+-} =& \frac{2}{\beta}\sum_{\vec{k}\in SBZ}\ln\Bigg(\\ &\frac{\sinh\left(\frac{\beta}{2}\left([B+2D|J|(\bar{m}+\Delta\tilde{m}_0.B)]^2-\left[2D|J|\gamma_{\vec{k}}(\bar{m}+\Delta\tilde{m}_0.B)\right]^2\right)^{1/2}\right)}{\sinh\left(\frac{\beta}{2}\left[B+2D|J|(\bar{m}+\Delta\tilde{m}_0.B)\right]\right)}\Bigg)\end{aligned} \tag{4.63}$$

The magnetization m on site i is the sum of a mean-field contribution $\bar{m} = -\frac{1}{\beta}\frac{\partial ln\mathcal{Z}_{MF}}{\partial B^z}$, a transverse contribution $\delta m_{+-} = -\frac{1}{\beta}\frac{\partial ln\mathcal{Z}_{+-}}{\partial B^z}$ and a longitudinal contribution $\delta m_{zz} = -\frac{1}{\beta}\frac{\partial ln\mathcal{Z}_{zz}}{\partial B^z}$. For a small magnetic field $\vec{B}$ a linear approximation leads to $m = \bar{m} + \delta m_{zz} + \delta m_{+-}$ where

$$\bar{m} = \frac{1}{2}\tanh\frac{\beta}{2}D|J|\bar{m} \tag{4.64}$$

$$\delta m_{zz} = -\frac{1}{\mathcal{N}\beta}\sum_{\vec{k}\in SBZ}\frac{8\bar{m}\Delta\tilde{m}_0\left(1-4\bar{m}^2\right)\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2}{\left[1-\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2\left(1-4\bar{m}^2\right)^2\right]} \tag{4.65}$$

$$\begin{aligned}\delta m_{+-} =& \frac{(1+2D|J|\Delta\tilde{m}_0)}{4\bar{m}}\\ &-\frac{1}{\mathcal{N}}\sum_{\vec{k}\in SBZ}\frac{\left(1+2D|J|\Delta\tilde{m}_0(1-\gamma_{\vec{k}}^2)\right)}{\sqrt{1-\gamma_{\vec{k}}^2}}\frac{1}{\left[\tanh\left(\beta D|J|\bar{m}\sqrt{1-\gamma_{\vec{k}}^2}\right)\right]}\end{aligned} \tag{4.66}$$

$\mathcal{N}$ is the number of spin-1/2 sites, $\Delta\tilde{m}_0 = \frac{\frac{\beta}{4}\left(1-4.\bar{m}^2\right)}{1-\frac{\beta}{2}D|J|(1-4.\bar{m}^2)}$ and $\gamma_{\vec{k}} = \frac{1}{D}\sum_{\vec{\eta}}\cos(\vec{k}.\vec{\eta})$ as defined in section 4.2.

At low temperature ($T\to 0$) it is seen that the magnetization goes over to the corresponding spin-wave expression [38, 51, 36, 9] and reads

$$m = 1-\frac{1}{\mathcal{N}}\sum_{\vec{k}\in SBZ}\frac{1}{\tanh\left(\frac{\beta D|J|}{2}\sqrt{1-\gamma_{\vec{k}}^2}\right)}.\frac{1}{\sqrt{1-\gamma_{\vec{k}}^2}} = \bar{m}+\delta m \tag{4.67}$$

where $\bar{m} = 1/2$ is the mean-field contribution and δm is generated by thermal and quantum fluctuations.

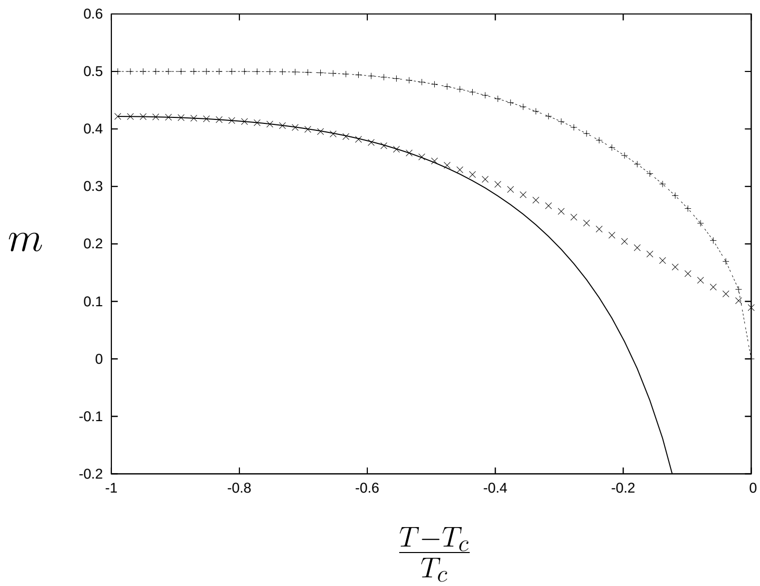


Figure 4.3: Magnetization in a 3D Heisenberg antiferromagnet cubic lattice. Dotted line : Mean-field magnetization, Dots : Spin-wave magnetization, Full line : One-loop corrected magnetization.

Figure 4.3 shows the magnetization m in the mean-field, the one-loop and the spin-wave approach (as given in section 4.2) for temperatures $T \leq T_c$ where $T_c = D|J|/2$ corresponds to a critical point. One observes a sizable contribution of the quantum and thermal fluctuations generated by the loop contribution over the whole range of temperatures as well as an excellent and expected agreement between the quantum corrected and the spin-wave result at very low temperatures.

The magnetization shows a singularity in the neighbourhood of the critical point. This behaviour can be read from the analytical expressions of δm_{+-} and δm_{zz} and is generated by the $|\vec{k}| = 0$ mode which leads to $\gamma_{\vec{k}} = 1$ and by cancellation of $\bar{m}$. The Néel state mean-field approximation is a realistic description at very low T. With increasing temperature this is no longer the case. The chosen ansatz breaks a symmetry whose effect is amplified as the temperature increases and leads to the well-known divergence disease observed close to T_c. Hence if higher order contributions in the loop expansion cannot cure the singularity the Néel state antiferromagnetic ansatz does not describe the physical symmetries of the system at the mean-field level at temperatures in the neighbourhood of the critical point. Consequently it is not a pertinent mean-field approximation for the description of the system.

The discrepancy can be quantified by means of the quantity $\frac{|\Delta m|}{\bar{m}}$ where $\Delta m = m - \bar{m} = \delta m_{zz} + \delta m_{+-}$. Figure 4.4 shows the result. The relation $\frac{|\Delta m|}{\bar{m}} < 1$ (Ginzburg criterion) fixes a limit temperature T_{lim} above which the quantum and thermal fluctuations generate larger contributions than the mean-field. For $3D$ systems this leads to $T_{lim} \simeq 0.8 T_c$, for $2D$ systems the criterion is never satisfied except maybe for very low temperature , see figure 4.5.

The pathology is the stronger the smaller the space dimensionality. It is also easy

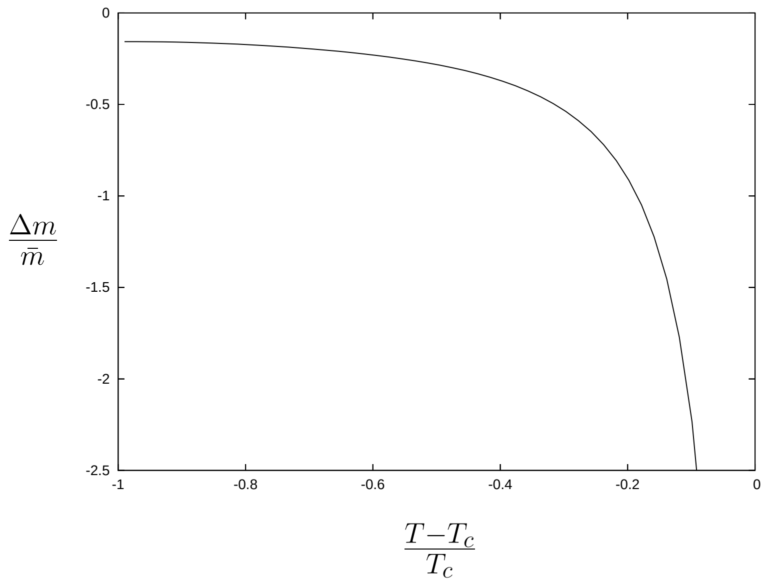


Figure 4.4: Ginzburg criterion $\frac{\Delta m}{\bar{m}}$ for the 3D Heisenberg model.

to see on the expression of the magnetization that, as expected, the contributions of the quantum fluctuations decrease with increasing D. As can be seen in the figure 4.5, the saddle point breaks down earlier in two than in three dimensions.

In fact, the Heisenberg model spin-wave spectrum shows a Goldstone mode as a consequence of the symmetry breaking by the Néel state. When $|\vec{k}|$ goes to zero

$$\omega_{\vec{k}} = ZDS\sqrt{1-\gamma_{\vec{k}}^2} \tag{4.68}$$

$$\lim_{\vec{k}\to\vec{0}} \omega_{\vec{k}} \sim |\vec{k}| \tag{4.69}$$

The zero mode destroys the long range order in 1D and 2D as expected from the Mermin-Wagner theorem [55].

4.5.4 The susceptibility : results

We consider the parallel susceptibility $\chi_\parallel$ which characterizes a magnetic system on which a uniform magnetic field is applied in the Oz direction. The expression of $\chi_\parallel$ decomposes again into three contributions

$$\chi_\parallel = -\frac{1}{\mathcal{N}}\frac{\partial^2 \mathcal{F}}{\partial B^2}\bigg|_{B=0} = \chi_{MF} + \chi_{zz} + \chi_{+-} \tag{4.70}$$

with

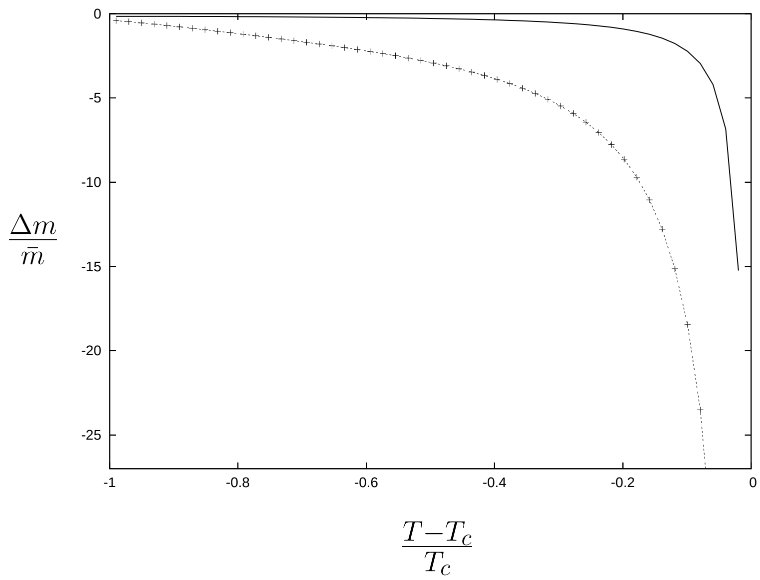


Figure 4.5: Comparison of the Ginzburg criterion applied to a 2D (dotted line) and 3D (full line) Heisenberg model.

$$\chi_{\|MF} = \Delta m_{\chi 0} = \frac{\frac{\beta}{4}\left(1-4\bar{m}^2\right)}{1+\frac{\beta}{2}D|J|\left(1-4\bar{m}^2\right)} \tag{4.71}$$

$$\chi_{\|zz} = -\frac{1}{\mathcal{N}\beta}\sum_{\vec{k}\in SBZ}\frac{8\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2 \Delta m_{\chi 0}^2\left(1+4\bar{m}^2\right)}{\left[1-\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2\left(1-4\bar{m}^2\right)^2\right]} \tag{4.72}$$

$$\chi_{\|+-} = \frac{1}{\mathcal{N}}\sum_{\vec{k}\in SBZ}\Bigg\{-\frac{1}{2}\frac{\beta\left(1-2D|J|\Delta m_{\chi 0}\right)^2}{\sinh^2\left(\beta D|J|\bar{m}\right)} \tag{4.73}$$

$$+\frac{1}{\sinh^2\left(\beta D|J|\bar{m}\sqrt{1-\gamma_{\vec{k}}^2}\right)} \tag{4.74}$$

$$\left[\frac{\beta}{2}\left(1-2D|J|\Delta m_{\chi 0}\right)^2-\beta\left(D|J|\Delta m_{\chi 0}\gamma_{\vec{k}}\right)^2\frac{\sinh 2\beta D|J|\bar{m}\sqrt{1-\gamma_{\vec{k}}^2}}{\beta D|J|\bar{m}\sqrt{1-\gamma_{\vec{k}}^2}}\right]\Bigg\} \tag{4.75}$$

The behaviour of $\chi_{\|}$ is shown in Figure 4.6 where we compare the mean-field, spin-wave and the one-loop corrected contributions for a system on a 3 D cubic lattice. One observes again a good agreement between the quantum corrected and the spin wave expressions at low temperatures. For higher temperatures the curves depart from each other as expected. The mean-field contribution remains in qualitative agreement with the total contribution.

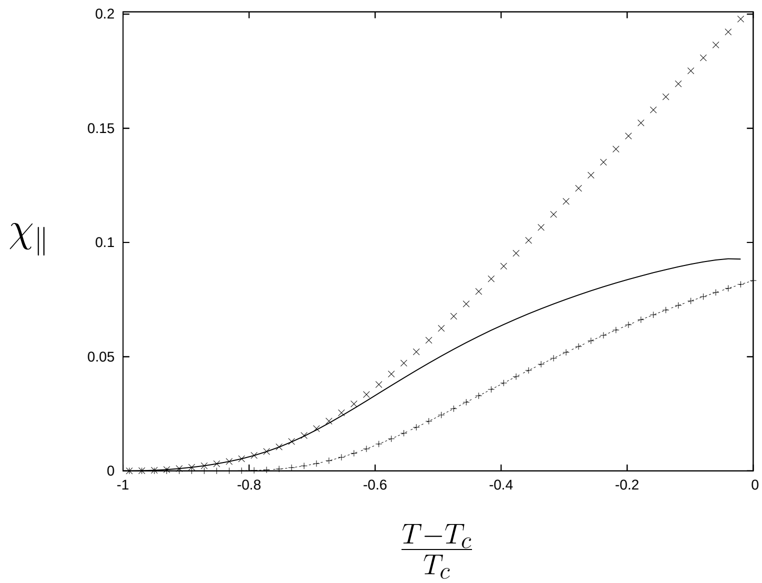


Figure 4.6: Parallel magnetic susceptibility at 3D for the Heisenberg model. Dots : Spin-wave susceptibility. Dotted line : Mean-field susceptibility $\chi_{\| MF}$. Full line : total susceptibility $(\chi_{\| MF} + \delta\chi_{\|})$.

4.6 The XXZ-model

To shed light on the fluctuations created by the symmetry breaking on an Heisenberg model when a Néel state is used as a mean-field state we add an anisotropic term $-\frac{J}{2}(1+\delta)S_i^z S_j^z$. In this case we consider a so called XXZ-model. The corresponding Hamiltonian of the system can be written

$$H^{XXZ} = -\frac{J}{2}\sum_{<ij>}\left(S_i^x S_j^x + S_i^y S_j^y + (1+\delta)S_i^z S_j^z\right) \tag{4.76}$$

where δ governs the anisotropy. The self-consistent mean-field magnetization of the XXZ-model reads

$$\bar{m} = \frac{1}{2}\tanh\frac{\beta}{2}D|J(1+\delta)|\bar{m} \tag{4.77}$$

Following the same steps as for the Heisenberg model we can compute the linear response of the system to the application of a magnetic field B_i in the direction of the Oz axis. The corresponding response to the mean-field magnetization $\bar{m}_i = (-1)^i\bar{m} + \Delta\tilde{m}_{XXZ}.B_i$ reads

$$\Delta\tilde{m}_{XXZ} = \frac{\frac{\beta}{4}\left(1 - 4.\bar{m}^2\right)}{1 - \frac{\beta}{2}D|J(1+\delta)|\left(1 - 4.\bar{m}^2\right)} \tag{4.78}$$

The magnetization is derived from the free energy given in the appendix C and reads

$$m = \bar{m} + \delta m_{zz} + \delta m_{+-} \tag{4.79}$$

where

$$\bar{m} = -\frac{1}{\mathcal{N}}\frac{\partial \mathcal{F}_{MF}}{\partial B}\bigg|_{B=0} = \frac{1}{2}\tanh\frac{\beta}{2}D|J(1+\delta)|\bar{m} \tag{4.80}$$

$$\begin{aligned}\delta m_{zz} &= -\frac{1}{\mathcal{N}}\frac{\partial \mathcal{F}_{zz}}{\partial B}\bigg|_{B=0} \\ &= -\frac{1}{\mathcal{N}\beta}\sum_{\vec{k}\in SBZ}\frac{8.\bar{m}\Delta\tilde{m}_{XXZ}\left(1-4\bar{m}^2\right)\left(\frac{\beta D|J(1+\delta)|\gamma_{\vec{k}}}{2}\right)^2}{\left[1-\left(\frac{\beta D|J(1+\delta)|\gamma_{\vec{k}}}{2}\right)^2\left(1-4\bar{m}^2\right)\right]}\end{aligned} \tag{4.81}$$

$$\begin{aligned}\delta m_{+-} &= -\frac{1}{\mathcal{N}}\frac{\partial \mathcal{F}_{+-}}{\partial B}\bigg|_{B=0} \\ &= \frac{(1+2D|J(1+\delta)|\Delta\tilde{m}_{XXZ})}{4\bar{m}} \\ &\quad -\frac{1}{\mathcal{N}}\sum_{\vec{k}\in SBZ}\frac{\left(1+2D|J(1+\delta)|\Delta\tilde{m}_{XXZ}(1-\left(\frac{J}{J(1+\delta)}\gamma_{\vec{k}}\right)^2)\right)}{\sqrt{1-\left(\frac{1}{(1+\delta)}\gamma_{\vec{k}}\right)^2}} \\ &\quad \frac{1}{\left[\tanh\left(\beta D|J|\bar{m}\sqrt{1-\left(\frac{1}{1+\delta}\gamma_{\vec{k}}\right)^2}\right)\right]}\end{aligned} \tag{4.82}$$

$$\tag{4.83}$$

The critical temperature T_c^{XXZ} of the mean-field magnetization for the XXZ-model reads

$$T_c^{XXZ} = \frac{D|J(1+\delta)|}{2} \tag{4.84}$$

For the zero temperature the excitation spectrum of the spin-wave obtained from the previous magnetization expressions leads now to a finite $|\vec{k}| = 0$ energy $\omega_{\vec{k}}$

$$\omega_{\vec{k}} = ZDS\sqrt{1-\left(\frac{1}{1+\delta}\gamma_{\vec{k}}\right)^2} \tag{4.85}$$

$$\lim_{\vec{k}\to\vec{0}}\omega_{\vec{k}} \sim \sqrt{1-\left(\frac{1}{1+\delta}\right)^2\left(1-\frac{\vec{k}^2}{2D}\right)} \tag{4.86}$$

By examination the expressions show that the zero momentum mode is no longer responsible for a breakdown of the saddle point procedure near $T_c^{XXZ} = \frac{D|J(1+\delta)|}{2}$. However the magnetization of the XXZ-model remains infinite near T_c^{XXZ}. This is due to the common disease shared with the Heisenberg model that the mean-field magnetization appearing in the denominator of δm_{+-} goes to zero near the critical temperature. One sees that the mean-field Néel state solution makes only sense at low temperatures, that is for $T \lesssim T_{lim}$, whatever the degree of symmetry breaking induced by the mean-field ansatz.

One notices that the spectrum $\omega_{\vec{k}}$ no longer vanishes in the limit $\vec{k} \to 0$ when the anisotropic coupling $\delta \neq 0$. Since this is the case the transverse modes need a finite amount of energy to get excited. Thus they are not Goldstone modes by virtue of the Goldstone theorem [8, 29]. The Néel state does not break the $O(2)$ symmetry but only the discrete one Z_2 (in the anisotropy direction Oz) of the XXZ-model.

4.7 Summary and conclusions

In the present chapter we aimed to work out the expression of physical observables (magnetization and susceptibility) starting from a specific mean-field ansatz and including contribution up to first order in a loop expansion in order to investigate the effect of fluctuation corrections to mean-field contributions at gaussian approximation. The mean-field was chosen as a Néel state which is an *a priori* reasonable choice for spin systems described in terms of unfrustrated bipartite Heisenberg model. The results were compared to those obtained in the framework of spin-wave theory. The PFP does not qualitatively change the well known magnetic properties of the Heisenberg model. However it must be pointed out that strict site-occupation had never been taken into account. This work remedies to this lack and was published in [21].

The number of particles per site was fixed by means of an strict constraint implemented in the partition function. It has been shown elsewhere [9, 22] that this fact introduces a large shift of the critical temperature compared to the case where the constraint is generated through an ordinary Lagrange multiplier term.

At low temperature the magnetization and the magnetic susceptibility are close to the spin-wave value as expected, also in agreement with former work [9]. Quantum corrections are sizable at low temperatures. With increasing temperature increasing thermal fluctuations add up to the quantum fluctuations.

At higher temperature the fluctuation contributions of quantum and thermal nature grow to a singularity in the neighbourhood of the critical temperature. The assumption that the Néel mean-field contributes for a major part to the magnetization and the susceptibility is no longer valid. Approaching the critical temperature T_c the mean-field contribution to the magnetization goes to zero and strong diverging fluctuations are generated at the one-loop order. This behaviour is common to the Heisenberg and XXZ magnetization. In addition the Néel order breaks $SU(2)$ symmetry of the Heisenberg Hamiltonian inducing low momentum fluctuations near T_c which is not the case in the XXZ-model.

The influence of fluctuations decreases with the increase of the dimension D of the system due to the expected fact that the mean-field contribution increases relatively to the loop contribution.

In dimension $D = 2$ the magnetization verifies the Mermin and Wagner theorem [55] for $T \neq 0$, the fluctuations are larger than the mean-field contribution for any temperature. In a more realistic description another mean-field ansatz may be necessary in order to describe the correct physics. Indeed Ghaemi and Senthil [28] have shown with the help of a specific model that a second order phase transition from a Néel mean-field to an ASL (algebraic spin liquid) may be at work depending on the strength of interaction parameter which enter the Hamiltonian of the system. This confirms that another mean-field solution like ASL may be a better starting point than a Néel state when the temperature T increases.

Chapter 5

Mean-field ansatz for the $2d$ Heisenberg model

Contents

We consider ordered quantum spin systems at finite temperature in which each lattice site is occupied by one electron with a given spin. Such a configuration can be constructed by means of constraints imposed through the specific projection operation [66] which fixes the occupation in a strict sense. The constraint can also be implemented on the average by means of a Lagrange multiplier procedure [8]. It is the aim of the present chapter to confront these two approaches in the framework of Heisenberg-type models.

The description of strongly interacting quantum spin systems at finite temperature generally goes through a saddle point procedure which is a zeroth order approximation of the partition function. The so generated mean-field solution is aimed to provide a qualitatively realistic approximation of the exact solution.

However mean-field solutions are not unique. The implementation of a mean-field structure is for a large part subject to an educated guess which should rest on essential properties of the considered system, in particular its symmetries. This generates a major difficulty. A considerable amount of work on this point has been made and a huge litterature on the subject is available. In particular, systems which are described by Heisenberg-type models without frustration are seemingly well described by ferromagnetic or antiferromagnetic (AF) Néel states at temperature $T = 0$ [13, 12]. It may however no longer be the case for many systems which are of low-dimensionality ($d \leq 2$) and (or) frustrated [82, 56, 47]. These systems show specific features. An extensive analysis and discussion in space dimension $d = 2$ has recently been presented by Wen [80]. The competition between AF and chiral spin state order has been the object of very recent investigations in the framework of continuum quantum field approaches at $T = 0$ temperature, see [78, 34].

The reason for the specific behaviour of low-dimensional systems may qualitatively be related to the fact that low-dimensionality induces strong quantum fluctuations, hence disorder which destroys the AF order. This motivates a transcription of the Hamiltonian in terms of composite operators which we call "diffusons" and "cooperons" below, with the hope that the actual symmetries different from those which are generated by AF order are better taken into account at the mean-field level [8].

In the present work we aim to work out a strict versus average treatment of the site-occupation constraint on systems governed by Heisenberg-type Hamiltonians at the mean-field level, for different types of order. This original work was published in [22].

The outline of the chapter is the following. Section 5.1 is devoted to the confrontation of the magnetization obtained through this procedure with the result obtained by means of an average projection procedure in the framework of the mean-field approach characterized by a Néel state. The same confrontation is done in section 5.2 for the order parameter which characterizes the system when its Hamiltonian is written in terms of so called Abrikosov fermions [56, 8] in $d = 2$ space dimensions. In section 5.3 we show that the rigorous projection [66] is no longer applicable when the Hamiltonian is written in terms of composite "cooperon" operators.

5.1 Antiferromagnetic mean-field ansatz

5.1.1 Exact occupation procedure

In this subsection we repeat the main steps of the partition function derivation given in section (4.3) with a slight modification. Instead of integrating over the Grassmann variables we construct a mean-field Hamiltonian $\mathcal{H}_{MF}$ expressed in terms of the creation and annihilation fermion operators ($f^\dagger$ and f) and giving the same mean-field partition function $\mathcal{Z}_{MF}$ as if one integrates over the Grassmann variables. Another point is the fact that instead of using the modified Matsubara frequencies as shown in subsection 3.3.4 we keep the imaginary chemical potential as an explicit term outside of the time derivation ∂_τ.

Starting with the nearest-neighbour Heisenberg Hamiltonian defined in equation (4.3)

$$H = -J \sum_{<i,j>} \vec{S}_i.\vec{S}_j + \sum_i \vec{B}_i.\vec{S}_i \tag{5.1}$$

the partition function $\mathcal{Z}$ can be written in the form (3.39)

$$\begin{aligned}\mathcal{Z}^{(PFP)} &= \int_{\xi_{i,\sigma}(\beta)=-\xi_{i,\sigma}(0)} \mathcal{D}\xi e^{-\int_0^\beta d\tau \{\sum_{i,\sigma} \xi^*_{i,\sigma}(\tau)(\partial_\tau - \mu)\xi_{i,\sigma}(\tau) + H(\{\xi^*_{i,\sigma}(\tau),\xi_{i,\sigma}(\tau)\})\}} \\ &= \int \mathcal{D}\xi e^{-S(\{\xi^*_{i,\sigma},\xi_{i,\sigma}\})} \end{aligned}\tag{5.2}$$

where the $\{\xi^*_{i,\sigma}, \xi_{i,\sigma}\}$ are Grassmann variables corresponding to the operators $\{f^\dagger_{i\sigma}, f_{i\sigma}\}$ defined in section 3.1. These *Grassmann* variables depend on the imaginary time τ in the interval $[0, \beta]$. The action S is given by

$$S(\{\xi^*_{i,\sigma}, \xi_{i,\sigma}\}) = \int_0^\beta d\tau \sum_{i,\sigma} (\xi^*_{i,\sigma}(\tau)\partial_\tau \xi_{i,\sigma}(\tau) + \mathcal{H}^{(PFP)}(\{\xi^*_{i,\sigma}(\tau), \xi_{i,\sigma}(\tau)\})) \tag{5.3}$$

where

$$\mathcal{H}^{(PFP)}(\tau) = H(\tau) - \mu N(\tau) \tag{5.4}$$

and $N(\tau) \equiv \sum_{i,\sigma} \xi^*_{i,\sigma}(\tau)\xi_{i,\sigma}(\tau)$ is the particle number operator. μ is the imaginary chemical potential introduced in section 3.2 describing the Popov and Fedotov procedure. The Hubbard-Stratonovich (HS) transformation defined in subsection 4.3.1 which generates the vector fields $\{\vec{\varphi}_i\}$ leads to the partition function $\mathcal{Z}$ which can be written in the form

$$\mathcal{Z}^{(PFP)} = \int \mathcal{D}(\{\xi^*_{i,\sigma}, \xi_{i,\sigma}, \vec{\varphi}_i\}) e^{-\int_0^\beta d\tau [\sum_{i,\sigma} \xi^*_{i,\sigma}(\tau)\partial_\tau \xi_{i,\sigma}(\tau) + \mathcal{H}^{(PFP)}(\{\xi^*_{i,\sigma}, \xi_{i,\sigma}, \vec{\varphi}_i\})]} \tag{5.5}$$

In equation (5.5) the expression of $\mathcal{Z}$ is quadratic in the Grassmann variables $\{\xi^*_{i,\sigma}, \xi_{i,\sigma}\}$ over which the expression can be integrated. The remaining expression depends on the fields $\{\vec{\varphi}_i(\tau)\}$. A saddle point procedure decomposes $\vec{\varphi}_i(\tau)$ into a mean-field contribution and a fluctuating term

$$\vec{\varphi}_i(\tau) = \left(\vec{\bar{\varphi}}_i - \vec{B}_i\right) + \delta\vec{\varphi}_i(\tau) \tag{5.6}$$

where $\vec{\bar{\varphi}}_i$ are the constant solutions of the self-consistent equation

$$\vec{\bar{\varphi}}_i - \vec{B}_i = \frac{1}{2}\sum_j J_{ij}\frac{\vec{\bar{\varphi}}_j}{\|\vec{\bar{\varphi}}_j\|}\tanh\left(\frac{\beta\|\vec{\bar{\varphi}}_j\|}{2}\right) \tag{5.7}$$

as was shown in section 4.4 for equation (4.46).

The partition function takes the form

$$\mathcal{Z}^{(PFP)} = \mathcal{Z}^{(PFP)}_{MF}\int \mathcal{D}(\{\delta\vec{\varphi}_i\})e^{-S_{eff}(\{\delta\vec{\varphi}_i\})} \tag{5.8}$$

where the first term on the right hand side corresponds to the mean-field contribution and the second term describes the contributions of the quantum and thermal fluctuations.

In the following we focus our attention only to the mean-field part of the partition function

$$\mathcal{Z}^{(PFP)}_{MF} = e^{-S_{eff}}\Big|_{[\vec{\bar{\varphi}}]} = Tr\left[e^{-\beta\mathcal{H}^{(PFP)}_{MF}}\right] \tag{5.9}$$

where $\mathcal{H}^{(PFP)}_{MF}$ is the mean-field part of the Hamiltonian (5.4) and reads

$$\mathcal{H}^{(PFP)}_{MF} = -\frac{1}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) + \sum_i \vec{\bar{\varphi}}_i.\vec{S}_i - \mu\tilde{N} \tag{5.10}$$

where spin operators $\vec{S}_i$ are given by (3.2), $\left(J^{-1}\right)_{ij}$ is the inverse of the coupling matrix J_{ij} defined by (4.2) and $\tilde{N} = \sum_{i,\sigma} f^\dagger_{i\sigma}f_{i\sigma}$ is the number operator. The mean-field Hamiltonian (5.10) expressed in terms of the creation and annihilation operators $\{f^\dagger_{i,\sigma}, f_{i,\sigma}\}$ reads

$$\begin{aligned}\mathcal{H}^{(PFP)}_{MF} &= -\frac{1}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) \\ &+ \sum_i \begin{pmatrix} f^\dagger_{i,\uparrow} & f^\dagger_{i,\downarrow}\end{pmatrix}\begin{bmatrix}\left(-\mu + \frac{\bar{\varphi}^z_i}{2}\right) & \frac{\bar{\varphi}^-_i}{2} \\ \frac{\bar{\varphi}^+_i}{2} & -\left(\mu + \frac{\bar{\varphi}^z_i}{2}\right)\end{bmatrix}\begin{pmatrix} f_{i,\uparrow} \\ f_{i,\downarrow}\end{pmatrix}\end{aligned} \tag{5.11}$$

The mean-field Hamiltonian (5.11) can be diagonalized by means of a Bogoliubov transformation as shown in appendix D and leads to

$$
\begin{aligned}
\mathcal{H}_{MF}^{(PFP)} &= -\frac{1}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) \\
&+ \sum_i \left\{\omega_{i,(+)}^{(PFP)}\beta_{i,(+)}^{\dagger}\beta_{i,(+)} + \omega_{i,(-)}^{(PFP)}\beta_{i,(-)}^{\dagger}\beta_{i,(-)}\right\}
\end{aligned}
\tag{5.12}
$$

Fermion creation and annihilation operators $\{\beta_{i,(\pm)}^{\dagger}, \beta_{i,(\pm)}\}$ are linear combinations of operators $\{f_{i,\sigma}^{\dagger}, f_{i,\sigma}\}$ and the corresponding excitation energies $\omega_{i,(\pm)}^{(PFP)}$ reads

$$
\omega_{i,(\pm)}^{(PFP)} = \mu \pm \frac{\|\vec{\bar{\varphi}}_i\|}{2}
\tag{5.13}
$$

The partition is then easily worked out and reads

$$
\begin{aligned}
Z_{MF}^{(PFP)} &= i^{-\mathcal{N}} e^{\frac{1}{2}\beta\sum\limits_{ij} J_{ij}^{-1}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right)} \prod_i (1 + e^{-\beta\omega_{i,(+)}^{(PFP)}})(1 + e^{-\beta\omega_{i,(-)}^{(PFP)}}) \\
&= e^{\frac{1}{2}\beta\sum\limits_{ij} J_{ij}^{-1}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right)} \prod_i \cosh\left(\frac{\beta\|\vec{\bar{\varphi}}_i\|}{2}\right)
\end{aligned}
\tag{5.14}
$$

and the free energy is given by the expression

$$
\mathcal{F}_{MF}^{(PFP)} = -\frac{1}{\beta}\ln \mathcal{Z}_{MF} = -\frac{1}{2}\sum_{ij} J_{ij}^{-1}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) - \frac{1}{\beta}\sum_i \ln 2\cosh\left(\frac{\beta\|\vec{\bar{\varphi}}_i\|}{2}\right)
\tag{5.15}
$$

Going through the same steps as in section 4.5.1 the local mean-field magnetization $\left\{\vec{\bar{m}}_i\right\}$ is obtained from

$$
\vec{\bar{m}}_i = -\frac{\partial \mathcal{F}_{MF}^{(PFP)}}{\partial \vec{B}_i}\bigg|_{\{\vec{B}_i = \vec{0}\}}
\tag{5.16}
$$

and is related to the $\{\vec{\bar{\varphi}}_i\}$'s by

$$
\vec{\bar{m}}_i = \frac{1}{2}\frac{\vec{\bar{\varphi}}_i}{\bar{\varphi}_i}\tanh\left[\frac{\beta\bar{\varphi}_i}{2}\right]
\tag{5.17}
$$

and by virtue of the relations (4.55) and (4.56) one gets the self-consistent equation for the $\{\vec{\bar{m}}_i\}$

$$\vec{\bar{m}}_i = \frac{2}{\beta}\sum_j J_{ij}^{-1} \tanh^{-1}\left(2\bar{m}_j\right) \frac{\vec{\bar{m}}_j}{\|\vec{\bar{m}}_j\|} \tag{5.18}$$

If the local fields $\{\vec{B}_i\}$ are oriented along a fixed direction $\vec{e}_z$, $\vec{\bar{m}}_i = \bar{m}_i\vec{e}_z$, the magnetizations are the solutions of the self-consistent equations

$$\bar{m}_i = \frac{1}{2}\tanh\left(\frac{\beta\sum\limits_j J_{ij}\bar{m}_j}{2}\right) \tag{5.19}$$

5.1.2 Lagrange multiplier approximation

In section 3.1 we introduced the projector (3.18)

$$\tilde{P}_i = \int \mathcal{D}\lambda_i e^{\lambda_i(\sum\limits_\sigma f_{i\sigma}^\dagger f_{i\sigma}-1)} \tag{5.20}$$

which allows to fix to one the number of spin-1/2 per lattice site. Similarly to the preceding case in which the Popov and Fedotov imaginary chemical potential was used one can introduce the one-particle site occupation by means of a Lagrange procedure. In order to do that one has to replace the Popov and Fedotov projector $\tilde{P} = \frac{1}{i^{\tilde{N}}}e^{i\frac{\pi}{2}\tilde{N}}$ by (3.18). The Hamiltonian $\mathcal{H}$ then reads

$$\mathcal{H}^{(\lambda)} = \frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i.\vec{S}_j + \sum_i \vec{B}_i.\vec{S}_i + \sum_i \lambda_i(n_i - 1) \tag{5.21}$$

where λ_i is a variational parameter and $\{n_i = \sum\limits_\sigma f_{i\sigma}^\dagger f_{i\sigma}\}$ are particle number operators.

Following the same lines as in section 5.1.1 with the help of a Hubbard-Stratonovich transformation and a Bogoliubov transformation as shown in appendix D the mean-field partition function $\mathcal{Z}_{MF}^{(\lambda)}$ can be worked out

$$Z_{MF}^{(\lambda)} = e^{-\frac{1}{2}\beta\sum\limits_{i,j} J_{ij}^{-1}\left(\vec{\varphi}_i-\vec{B}_i\right)\left(\vec{\varphi}_j-\vec{B}_j\right)-\mathcal{N}\lambda} \prod_i (1+e^{-\beta\omega_{i,(+)}^\lambda})(1+e^{-\beta\omega_{i,(-)}^\lambda}) \tag{5.22}$$

with

$$\omega_{i,(+)}^\lambda = \lambda + \frac{\|\vec{\varphi}_j\|}{2} \tag{5.23}$$

$$\omega_{i,(-)}^\lambda = \lambda - \frac{\|\vec{\varphi}_j\|}{2} \tag{5.24}$$

The parameter λ is fixed through a minimization of the free energy with respect to λ

$$\left.\frac{\partial \mathcal{F}_{MF}^{(\lambda)}}{\partial \lambda_i}\right|_{\{\lambda_i=\lambda\}} = 0 \tag{5.25}$$

The minimization shows that the extremum solution is obtained for $\lambda = 0$ and

$$\mathcal{F}_{MF}^{(\lambda)} = -\frac{1}{2}\sum_{i,j} J_{ij}^{-1}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) - \frac{2}{\beta}\sum_i \ln 2\cosh\left(\frac{\beta\|\vec{\bar{\varphi}}_i\|}{4}\right) \tag{5.26}$$

which is different from the expression of equation (5.15) by a factor 1/2 in the argument of the cosh term.

The magnetization can be obtained in the same way as done in subsection 5.1.1. One obtains

$$\bar{m}_i^{(\lambda=0)} = \frac{1}{2}\tanh\left(\frac{\beta\sum_j J_{ij}\bar{m}_j^{(\lambda=0)}}{4}\right) \tag{5.27}$$

which is again different from the expression obtained in the case of a rigorous projection, see equation (5.19).

The uniform solutions $\bar{m}_i^{(PFP)} = (-1)^i \bar{m}^{(PFP)}$ and $\bar{m}_i^{(\lambda=0)} = (-1)^i \bar{m}^{(\lambda=0)}$ for $J_{ij} = J \sum_{\vec{\eta}\in\{\vec{a}_1,\ldots,\vec{a}_D\}} \delta\left(\vec{r}_i - \vec{r}_j \pm \vec{\eta}\right)$ have been calculated by solving the selfconsistent equations (5.19) and (5.27). The results are shown in figure (5.1). It is seen that the treatment of the site-occupation affects sizably the quantitive behaviour of observables. In particular it shifts the location of the critical temperature T_c by a factor 2. Such a strong effect has already been observed on the behaviour of the specific heat, see refs. [9, 42].

5.2 Spin state mean-field ansatz in 2d

In $2d$ space the Heisenberg Hamiltonian given by

$$H = -J\sum_{<i,j>} \vec{S}_i.\vec{S}_j \tag{5.28}$$

can be written in terms of composite non-local operators $\{\mathcal{D}_{ij}\}$ ("diffusons") [8] defined as

$$\mathcal{D}_{ij} = f_{i,\uparrow}^\dagger f_{j,\uparrow} + f_{i,\downarrow}^\dagger f_{j,\downarrow} \tag{5.29}$$

If the coupling strengths are fixed as

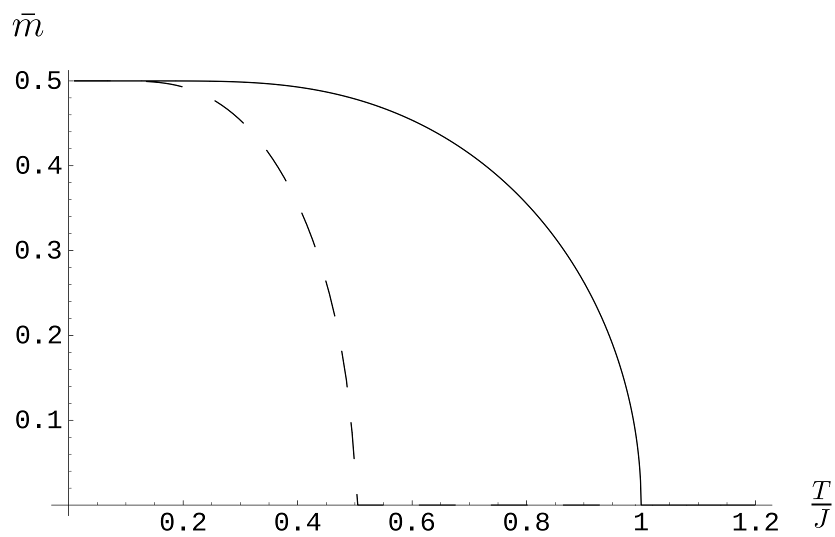


Figure 5.1: Magnetization vs. reduced temperature $t = T/|J|$. Full line: exact site-occupation. Dashed line: average site-occupation.

$$J_{ij} = J \sum_{\vec{\eta}} \delta\left(\vec{r}_i - \vec{r}_j \pm \vec{\eta}\right) \tag{5.30}$$

where $\vec{\eta}$ is a lattice vector $\{a_1, a_2\}$ in the $\vec{Ox}$ and $\vec{Oy}$ directions the Hamiltonian takes the form

$$H = -J \sum_{<ij>} \left(\frac{1}{2}\mathcal{D}^{\dagger}_{ij}\mathcal{D}_{ij} - \frac{n_i}{2} + \frac{n_i n_j}{4}\right) \tag{5.31}$$

where i and j are nearest neighbour sites.

The number operator products $\{n_i n_j\}$ in Eq.(5.31) are quartic in terms of creation and annihilation operators in Fock space. In principle the formal treatment of these terms requires the introduction of a mean-field procedure. One can however show that the presence of this term has no influence on the results obtained from the partition function. Indeed these terms lead to a constant quantity under the exact site-occupation constraint and hence are of no importance for the physics described by the Hamiltonian (5.31). As a consequence we leave it out from the beginning as well as the contribution corresponding to the $\{n_i\}$ terms.

5.2.1 Exact occupation procedure

Starting with the Hamiltonian

$$\mathcal{H}^{(PFP)} = -\frac{J}{2} \sum_{<ij>} \mathcal{D}^{\dagger}_{ij}\mathcal{D}_{ij} - \mu N \tag{5.32}$$

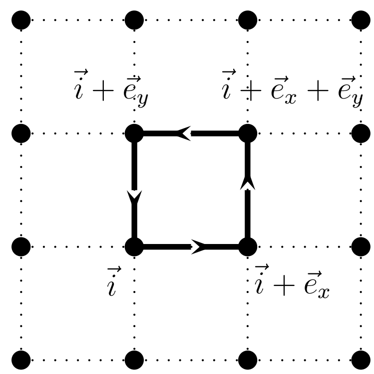


Figure 5.2: Plaquette (□) on a two dimensionnal spin lattice

the partition function $\mathcal{Z}$ can be written in the form (5.2) and the Hamiltonian in the form (5.4). A Hubbard-Stratonovich transformation on the corresponding functional integral partition function in which the action contains the occupation number operator as seen in equation (5.3) eliminates the quartic contributions generated by equation (5.29) and introduces the mean-fields $\{\Delta_{ij}\}$. The Hamiltonian takes then the form

$$\mathcal{H}^{(PFP)} = \frac{2}{|J|}\sum_{<ij>}\bar{\Delta}_{ij}\Delta_{ij} + \sum_{<ij>}\left[\bar{\Delta}_{ij}\mathcal{D}_{ij} + \Delta_{ij}\mathcal{D}^{\dagger}_{ij}\right] - \mu N \tag{5.33}$$

The fields $\{\Delta_{ij}\}$ and their complex conjugates $\{\bar{\Delta}_{ij}\}$ can be decomposed into a mean-field contribution and a fluctuation term

$$\Delta_{ij} = \Delta_{ij}^{MF} + \delta\Delta_{ij} \tag{5.34}$$

The field Δ_{ij}^{MF} can be chosen as a complex quantity $\Delta_{ij}^{MF} = |\Delta_{ij}^{MF}|e^{i\phi_{ij}^{MF}}$.

The phase ϕ_{ij}^{MF} is fixed in the following way. Consider a square plaquette $\square \equiv \left(\vec{i}, \vec{i}+\vec{e}_x, \vec{i}+\vec{e}_x+\vec{e}_y, \vec{i}+\vec{e}_y\right)$ where $\vec{e}_x$ and $\vec{e}_y$ are the unit vectors along the directions $\vec{Ox}$ and $\vec{Oy}$ starting from site $\vec{i}$ on the lattice as shown in figure (5.2). On this plaquette we define

$$\phi = \sum_{(ij)\in\square}\phi_{ij}^{MF} \tag{5.35}$$

which is taken to be constant. If the gauge phase ϕ_{ij}^{MF} fluctuates in such a way that ϕ stays constant the average of Δ_{ij}^{MF} will be equal to zero in agreement with Elitzur's theorem [26]. In order to guarantee the $SU(2)$ invariance of the mean-field Hamiltonian along the plaquette we follow [2, 7, 49, 54, 80] and introduce

$$\phi_{ij} = \begin{cases} e^{i.\frac{\pi}{4}(-1)^i}, \text{if } \vec{r}_j = \vec{r}_i + \vec{e}_x \\ e^{-i.\frac{\pi}{4}(-1)^i}, \text{if } \vec{r}_j = \vec{r}_i + \vec{e}_y \end{cases} \tag{5.36}$$

where $\vec{e}_x$ and $\vec{e}_y$ join the site i to its nearest neighbours j. Then the total flux through the fundamental plaquette is such that $\phi = \pi$ which guarantees that the $SU(2)$ symmetry of the plaquette is respected [53].

At the mean-field level the partition function reads

$$\mathcal{Z}_{MF}^{(PFP)} = e^{-\beta \mathcal{H}_{MF}^{(PFP)}} \tag{5.37}$$

where

$$\mathcal{H}_{MF}^{(PFP)} = \frac{2}{|J|} \sum_{<ij>} \bar{\Delta}_{ij}^{MF}.\Delta_{ij}^{MF} + \sum_{<ij>} \left[\bar{\Delta}_{ij}^{MF} \mathcal{D}_{ij} + \Delta_{ij}^{MF} \mathcal{D}_{ij}^{\dagger} \right] - \mu N \tag{5.38}$$

After a Fourier transformation the Hamiltonian (5.38) takes the form

$$\mathcal{H}_{MF}^{(PFP)} = \mathcal{N} z \frac{\Delta^2}{|J|} + \sum_{\vec{k} \in SBZ} \sum_{\sigma} \left(f_{\vec{k},\sigma}^{\dagger} \; f_{\vec{k}+\vec{\pi},\sigma}^{\dagger} \right) \left[\widetilde{\mathcal{H}}^{(PFP)} \right] \begin{pmatrix} f_{\vec{k},\sigma} \\ f_{\vec{k}+\vec{\pi},\sigma} \end{pmatrix} \tag{5.39}$$

with

$$\left[\widetilde{\mathcal{H}}^{(PFP)} \right] = \begin{bmatrix} -\mu + \Delta \cos \frac{\pi}{4} z \gamma_{k_x,k_y} & -i\Delta \sin \frac{\pi}{4} z \gamma_{k_x,k_y+\pi} \\ +i\Delta \sin \frac{\pi}{4} z \gamma_{k_x,k_y+\pi} & -\mu - \Delta \cos \frac{\pi}{4} z \gamma_{k_x,k_y} \end{bmatrix} \tag{5.40}$$

where $\Delta \equiv |\Delta^{MF}|$. The Spin Brillouin Zone (SBZ) covers half of the Brillouin Zone (see figure 4.2 in subsection 4.2.2). The $\gamma_{\vec{k}}$'s are defined by

$$\gamma_{\vec{k}} = \frac{1}{z} \sum_{\vec{\eta}} e^{i\vec{k}.\vec{\eta}} = \frac{1}{2} \left(\cos k_x a_1 + \cos k_y a_2 \right) \tag{5.41}$$

where $z = 4$ is the coordination and $\mathcal{N}$ the number of sites. a_1 and a_2 are the lattice parameters in direction $\vec{Ox}$ and $\vec{Oy}$. The lattice parameters are not important for our study. We renormalize the wave vector $\vec{k}$ by the relations $k_x = k_x.a_1$ and $k_y = k_y.a_2$ as shown in appendix B. The momenta $\{\vec{k}\}$ act in the first half Brillouin zone (spin Brillouin zone).

Performing a Bogolioubov transformation which diagonalizes the remaining expression (5.40) in Fourier space leads to

$$\mathcal{H}_{MF}^{(PFP)} = \frac{\mathcal{N} z \Delta^2}{|J|} + \sum_{\vec{k},\sigma} \left[\omega_{(+),\vec{k},\sigma}^{(PFP)} \beta_{(+),\vec{k},\sigma}^{\dagger} \beta_{(+),\vec{k},\sigma} + \omega_{(-),\vec{k},\sigma}^{(PFP)} \beta_{(-),\vec{k},\sigma}^{\dagger} \beta_{(-),\vec{k},\sigma} \right] \tag{5.42}$$

The transformation is worked out in appendix D.2. The eigenenergies $\omega^{(PFP)}_{(+),\vec{k},\sigma}$ and $\omega^{(PFP)}_{(-),\vec{k},\sigma}$ are given by

$$\omega^{(PFP)}_{(+),\vec{k},\sigma} = -\mu + 2\Delta[cos^2(k_x) + cos^2(k_y)]^{1/2} \tag{5.43}$$

and similarly

$$\omega^{(PFP)}_{(-),\vec{k},\sigma} = -\mu - 2\Delta[cos^2(k_x) + cos^2(k_y)]^{1/2} \tag{5.44}$$

The partition function Z_{MF} has the same structure as the corresponding partition function in equation (5.14) and the free energy is given by

$$\mathcal{F}^{(PFP)}_{MF} = \frac{\mathcal{N} z \Delta^2}{|J|} - \frac{1}{\beta}\sum_{\vec{k},\sigma} \ln\left(2\cosh\beta\Delta\varepsilon_{\vec{k}}\right) \tag{5.45}$$

with

$$\varepsilon_{\vec{k}} = 2\left[cos^2(k_x) + cos^2(k_y)\right]^{1/2} \tag{5.46}$$

Finally the variation of $\mathcal{F}_{MF}$ with respect to Δ leads to the self-consistent mean-field equation

$$\tilde{\Delta}^{(PFP)} = \frac{1}{2\mathcal{N}}\sum_{\vec{k},\sigma}\varepsilon_{\vec{k}} \tanh\left(\frac{\beta|J|\varepsilon_{\vec{k}}\tilde{\Delta}^{(PFP)}}{z}\right) \tag{5.47}$$

with $\tilde{\Delta}^{(PFP)} = z\Delta/|J|$ which fixes Δ.

5.2.2 Lagrange multiplier approximation

Similarly to equation (5.21) one may introduce a Lagrange constraint and write

$$\mathcal{H}^{(\lambda)} = \frac{2}{|J|}\sum_{<ij>}\bar{\Delta}_{ij}\Delta_{ij} + \sum_{<ij>}\left(\bar{\Delta}_{ij}\mathcal{D}_{ij} + \Delta_{ij}\mathcal{D}^{\dagger}_{ij}\right) + \sum_{i}\lambda_i\left(n_i - 1\right) \tag{5.48}$$

In the mean-field approximation one have

$$\lambda_i = \lambda \tag{5.49}$$

and after a Bogoliubov transformation as for equation (5.42) the mean-field Hamiltonian reads

$$H_{MF}^{(\lambda)} = \frac{\mathcal{N} z \Delta^2}{|J|} + \sum_{\vec{k},\sigma} \left(\omega^{(\lambda)}_{(+),\vec{k},\sigma} \beta^\dagger_{(+)\vec{k},\sigma} \beta_{(+)\vec{k},\sigma} + \omega^{(\lambda)}_{(-),\vec{k},\sigma} \beta^\dagger_{(-)\vec{k},\sigma} \beta_{(-)\vec{k},\sigma} \right) \tag{5.50}$$

with the eigenenergies

$$\omega^{(\lambda)}_{(+),\vec{k},\sigma} = \lambda + 2\Delta[cos^2(k_x) + cos^2(k_y)]^{1/2} \tag{5.51}$$

and similarly

$$\omega^{(\lambda)}_{(-),\vec{k},\sigma} = \lambda - 2\Delta[cos^2(k_x) + cos^2(k_y)]^{1/2} \tag{5.52}$$

The expression of the free energy is now given by

$$\mathcal{F}_{MF}^{(\lambda)} = -\mathcal{N}\lambda + \frac{\mathcal{N} z \Delta^2}{|J|} - \frac{1}{\beta} \sum_{\vec{k},\sigma} \ln \left[1 + e^{-\beta \omega^{(\lambda)}_{(+),\vec{k},\sigma}} \right] \left[1 + e^{-\beta \omega^{(\lambda)}_{(-),\vec{k},\sigma}} \right] \tag{5.53}$$

As was shown in subsection 5.1.2 the minimization of this expression in terms of λ delivers the solution $\lambda = 0$ and

$$\mathcal{F}_{MF}^{(\lambda)} = +\frac{\mathcal{N} z \Delta^2}{|J|} - \frac{1}{\beta} \sum_{\vec{k},\sigma} 2 \ln \left(2 \cosh \frac{\beta \Delta \varepsilon_{\vec{k}}}{2} \right) \tag{5.54}$$

where $\varepsilon_{\vec{k}}$ is given by equation (5.46).

The variation of $\mathcal{F}_{MF}^{(\lambda)}$ with respect to Δ leads to the self-consistent mean-field equation

$$\tilde{\Delta}^{(\lambda)} = \frac{1}{\mathcal{N}} \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} \tanh \left(\frac{\beta |J| \varepsilon_{\vec{k}} \tilde{\Delta}^{(\lambda)}}{2z} \right) \tag{5.55}$$

with $\tilde{\Delta}^{(\lambda)} = z\Delta/|J|$.

Expressions in equation (5.54) and equation (5.55) should be compared to the expressions obtained in equation (5.45) and equation (5.47). Figure 5.3 shows the behaviour of $\tilde{\Delta}$ for the two different treatments of site-occupation on the lattice. The exact occupation procedure compared to Lagrange multiplier approximation doubles the critical temperature of the order parameter $\tilde{\Delta}$ as was shown in section 5.1 and in [9] for the Néel state.

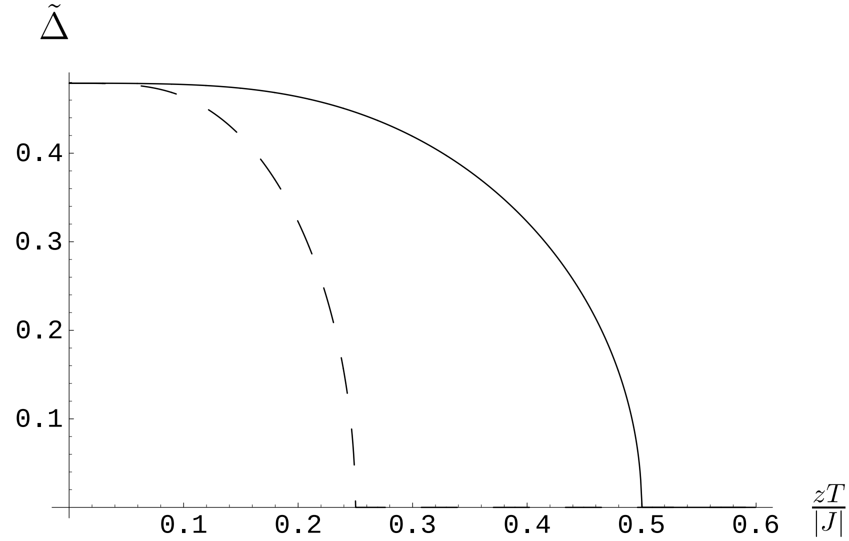


Figure 5.3: $\tilde{\Delta}$ vs. reduced temperature $\tilde{t} = zT/|J|$. Full line: exact site-occupation $\tilde{\Delta}^{(PFP)}$. Dashed line: average site ocupation $\tilde{\Delta}^{(\lambda)}$.

5.3 Cooperon mean-field ansatz

Starting from the Hamiltonian

$$H = -|J| \sum_{<i,j>} \vec{S}_i \vec{S}_j \tag{5.56}$$

one can introduce a further set of non-local composite operators $\{\mathcal{C}_{ij}\}$ (”cooperons”)

$$\mathcal{C}_{ij} = f_{i,\uparrow} f_{j,\downarrow} - f_{i,\downarrow} f_{j,\uparrow} \tag{5.57}$$

This leads to the expression

$$H = \frac{|J|}{2} \sum_{<i,j>} \left(\mathcal{C}^\dagger_{ij} \mathcal{C}_{ij} + \frac{n_i n_j}{2} \right) \tag{5.58}$$

where $n_i = \sum\limits_{\sigma} f^\dagger_{i,\sigma} f_{i,\sigma}$. As was explained in section 5.2 for the Hamiltonian composed of the operator $\mathcal{D}_{ij}$ the second term in the right hand side of equation (5.58) is quartic in the fermion creation and annihilation operator $f^\dagger, f$ hence one needs to use a Hubbard-Stratonovich transformation in order to reduce this term to a quadratic form. Calculations show that the second term is irrelevant. The solution of the self-consistent equations of the auxiliary field introduced by the Hubbard-Stratonovich procedure lead to $\{n_i = 1\}$.

5.3.1 Exact occupation procedure

As in the preceding cases it is possible to implement a Hubbard-Stratonovich procedure on the $\{\mathcal{C}_{ij}\}$ in such a way that the expresssion of the corresponding partition function gets quadratic in the fields $\{f_{i,\uparrow}, f_{i,\downarrow}\}$. The corresponding HS fields are $\{\Gamma_{ij}\}$ and

$$H = \frac{2}{|J|}\sum_{<i,j>} \bar{\Gamma}_{ij}\Gamma_{ij} + \sum_{<i,j>} \left(\bar{\Gamma}_{ij}\mathcal{C}_{ij} + \Gamma_{ij}\mathcal{C}^{\dagger}_{ij} \right) \tag{5.59}$$

Introducing the homogeneous mean-fields $\left\{\Gamma_{ij} = \Gamma = \bar{\Gamma}\right\}$, one gets in Fourier space

$$\mathcal{H}^{(PFP)}_{MF} = \mathcal{N}\frac{z\Gamma^2}{|J|} - \sum_{\vec{k}\in BZ,\sigma} \left[\mu f^{\dagger}_{\vec{k},\sigma} f_{\vec{k},\sigma} + \sigma \frac{z\Gamma\gamma_{\vec{k}}}{2} \left(f_{\vec{k},\sigma} f_{-\vec{k},-\sigma} - f^{\dagger}_{\vec{k},\sigma} f^{\dagger}_{-\vec{k},-\sigma} \right) \right] \tag{5.60}$$

with

$$\gamma_{\vec{k}} = \frac{1}{2}(cos k_x + cos k_y) \tag{5.61}$$

The second term in this expression is complex since $\mu = i\pi/2\beta$. In this representation it is not possible to find a **unitary** Bogolioubov transformation which diagonalizes H as shown in appendix D.3. Hence a rigorous implementation of the constraint on the particle number per site is not possible.

Reasons for this situation are the fact that the Hamiltonian contains terms with two particles with opposite spin created or annihilated on the same site which is incompatible with the fact that such configurations are not allowed in the present scheme. Terms of this type are typical in mean-field pairing Hamiltonians which lead to a non-conservation of the number of particles of the system as for the BCS-normal transition.

5.3.2 Lagrange multiplier approximation

If the sites are occupied by one electron in the average the Lagrange procedure works opposite to the exact procedure. Here a Bogoliubov transformation can be defined and used to diagonalize the mean-field Hamiltonian. We do not develop the derivation of the mean-field physical behaviour here since it has been done elsewhere [7, 8, 51].

5.4 Summary and conclusions

In summary we have shown that a strict constraint on the site-occupation of a lattice quantum spin system described by Heisenberg-type models shows a sizable quantitative different localization of the critical temperature when compared with the outcome of an average occupation constraint. Consequently it generates sizable effects on the behaviour of order parameters, see also reference [22]. With exact site-occupation the transition temperature of antiferromagnetic Néel and spin states order parameters are twice as large as the critical temperature one gets from an average Lagrange multiplier method.

Opposite to the average procedure the exact occupation procedure can not be used on cooperon states mean-field Hamiltonian. Cooperon are BCS pairs then destroy two quasi-particles in favor to create a new one which is a pair and then the number of particle are not concerved opposite to the exact occupation method. No fluctuations of the number of particles are tolerated by the exact occupation procedure.

Due to the complexity of quantum spin systems the choice of a physically meaningful mean-field may depend on the coupling strengths of the model which describes the systems [81]. A $specific$ mean-field solution may even be a naive way to fix the "classical" contribution to the partition function which may in fact contain a mixture of different types of states. As already mentioned many efforts have been and are done in order to analyze and overcome these problems by means of different arguments [34, 78, 80].

In a more realistic analysis one should of course take care of the contributions of quantum fluctuations which may be of overwhelming importance particularly in the vicinity of critical points. Chapter 6 study the implications of the phase flutuations around the π-flux mean-field state.

Chapter 6

Two-dimensional Heisenberg model and dynamical mass generation in QED_3 at finite temperature

Contents

A Néel ansatz is not necessarily a good candidate for the description of two dimensional quantum spin systems. We showed in chapter 4 that such an ansatz breaks the $SU(2)$ spin symmetry generating Goldstone bosons which destroy the Néel order. A better candidate seems to be the spin liquid ansatz since it keeps $SU(2)$ symmetry unaffected. For this reason in the following we concentrate us on the spin liquid phase.

Quantum Electrodynamics $QED_{(2+1)}$ is a common framework which can be used to describe strongly correlated systems such as quantum spin systems in 1 time and 2 space dimensions, as well as related specific phenomena like high-T_c superconductivity [27, 28, 50, 57]. A gauge field formulation of antiferromagnetic Heisenberg models in $d = 2$ space dimensions maps the initial action onto a QED_3 action for spinons [28, 57]. This description raises the problem of the mean-field solution and the correlated question of the confinement of test charges which may lead to the impossibility to determine the quantum fluctuation contributions through a loop expansion in this approach [32, 33, 62].

We consider here the π-flux state approach introduced by Affleck and Marston [2, 54]. The occupation of sites of the system by a single particle is generally introduced by means of a Lagrange multiplier procedure [8, 7]. In the present work we implement the strict site-occupation by means of constraints imposed through a specific projection operator which introduces the imaginary chemical potential proposed by Popov and Fedotov [66] for $SU(2)$ and modifies the Matsubara frequencies as explained in chapter 3.

Here we concentrate on the generation and behaviour of spinon mass which stems from the presence of a $U(1)$ gauge field. Appelquist et al. [5, 6] have shown that at zero temperature the originally massless fermion can acquire a dynamically generated mass when the number N of fermion flavors is lower than the critical value $N_c = 32/\pi^2$. Later Maris [52] confirmed the existence of a critical value $N_c \simeq 3.3$ below which the dynamical mass can be generated. Since we consider only spin-1/2 systems, $N = 2$ and hence $N < N_c$.

At finite temperature Dorey and Mavromatos [24] and Lee [48] showed that the dynamically generated mass vanishes at a temperature T larger than the critical one T_c.

We shall show below that the imaginary chemical potential introduced by Popov and Fedotov [66] modifies noticeably the effective potential between two charged particles and doubles the dynamical mass transition temperature, in agreement with former work at the same mean-field level [22]. This original work published in [23] leads to another work which is not directly related to the PFP and concerns the introduction of a Chern-Simons term in our theory [20].

The outline of the chapter is the following. In section 6.1 we give a definition of a spinon. In section 6.2 we derive the Lagrangian which couples a spinon field to a $U(1)$ gauge field. Section 6.3 is devoted to the comparison of the effective potential constructed with and without strict occupation constraint. In section 6.4 we present the calculation of the mass term using the Schwinger-Dyson equation of the spinon. Section 6.4 gives an outlook on the spin-charge separation phenomenon and confinement problems.

6.1 Definition of a Spinon

Electrons are particles with charge e and spin $S = 1/2$. Formally they can be defined by creation and annihilation operators $C^{\dagger}_{\vec{r},\sigma}$ and $C_{\vec{r},\sigma}$ at position $\vec{r}$ and spin projection $\sigma = \pm 1/2$. In this description the $t-J$ model which was largely studied for low-dimensional systems after the discovery of High-T_c superconductivity reads [4, 31, 35, 82]

$$H = -\sum_{ij}\sum_{\sigma} t_{ij} C^{\dagger}_{i,\sigma} C_{j,\sigma} + \sum_{ij} J_{ij} \vec{S}_i . \vec{S}_j \tag{6.1}$$

where t_{ij} is the so called hopping energy when the electrons jumps from j to site i and J_{ij} is the spin coupling matrix as defined in section 3.1.

It is believed that for a linear chain the $t-J$ model leads to the phenomenon of *spin-charge separation* for strong electronic correlations [43, 58]. Observation of spin-charge separation in one-dimensional materials such as $SrCuO_2$ confirms this belief [40]. In this framework the creation and annihilation operators $C^{\dagger}_{\vec{r},\sigma}$ and $C_{\vec{r},\sigma}$ are represented in terms of spinon $f^{\dagger}_{\vec{r},\sigma}$, $f_{\vec{r},\sigma}$, holon $h^{\dagger}_{\vec{r}}$, $h_{\vec{r}}$ and doublon $d^{\dagger}_{\vec{r}}$, $d_{\vec{r}}$ creation and annihilation operators and read [59]

$$\begin{aligned} C^{\dagger}_{\vec{r},\sigma} &= f^{\dagger}_{\vec{r},\sigma} h_{\vec{r}} + \varepsilon_{\sigma\sigma'} f_{\vec{r}\sigma'} d^{\dagger}_{\vec{r}} \\ C_{\vec{r}\sigma} &= f_{\vec{r},\sigma} h^{\dagger}_{\vec{r}} + \varepsilon_{\sigma\sigma'} f^{\dagger}_{\vec{r}\sigma'} d_{\vec{r}} \end{aligned} \tag{6.2}$$

where f fulfils fermion anticommutation, h and d fulfil commutation relations. $\varepsilon_{\sigma\sigma'}$ is the antisymmetric tensor. The transformation (6.2) is exact when the occupation lattice sites of these entities is controlled by a constraint and reads

$$h^{\dagger}_{\vec{r}} h_{\vec{r}} + f^{\dagger}_{\vec{r},\uparrow} f_{\vec{r},\uparrow} + f^{\dagger}_{\vec{r},\downarrow} f_{\vec{r},\downarrow} + d^{\dagger}_{\vec{r}} d_{\vec{r}} = 1 \tag{6.3}$$

corresponding to the fact that each lattice site can be occupied by a hole, a spin $\sigma =\uparrow$, a spin $\sigma =\downarrow$ or double occupancy. This description is the so called *slave-boson* method. One sees that holons and doublons are charge excitations while spinons are spin excitations of the electonic systems.

If the Popov and Fedotov procedure (PFP) is adopted holons and doublons are not allowed to live on the lattice and the constraint (6.3) reduces to

$$f^{\dagger}_{\vec{r},\uparrow} f_{\vec{r},\uparrow} + f^{\dagger}_{\vec{r},\downarrow} f_{\vec{r},\downarrow} = 1 \tag{6.4}$$

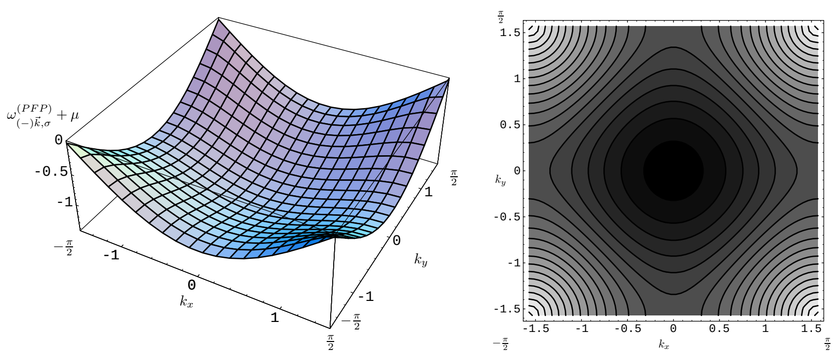
In this chapter since one considers the PFP only spinon entities are under consideration in our Heisenberg models describing cuprates in their insulating phase as explained in section 3.1.

6.2 The π-flux Dirac action of spinons

We have seen in section 5.2 that the Heisenberg Hamiltonian $H = -J \sum_{<i,j>} \vec{S}_i.\vec{S}_j$ can be expressed in terms of the diffuson operator $\{\mathcal{D}_{ij}\}$ and leads to the π-flux mean-field Hamiltonian

$$
\begin{aligned}
\mathcal{H}_{MF}^{(PFP)} &= \mathcal{N} z \frac{\Delta^2}{|J|} \\
+ \sum_{\vec{k} \in SBZ} \sum_{\sigma} & \begin{pmatrix} f^\dagger_{\vec{k},\sigma} & f^\dagger_{\vec{k}+\vec{\pi},\sigma} \end{pmatrix} \begin{bmatrix} -\mu + \Delta \cos\frac{\pi}{4} z \gamma_{k_x,k_y} & -i\Delta \sin\frac{\pi}{4} z \gamma_{k_x,k_y+\pi} \\ +i\Delta \sin\frac{\pi}{4} z \gamma_{k_x,k_y+\pi} & -\mu - \Delta \cos\frac{\pi}{4} z \gamma_{k_x,k_y} \end{bmatrix} \begin{pmatrix} f_{\vec{k},\sigma} \\ f_{\vec{k}+\vec{\pi},\sigma} \end{pmatrix}
\end{aligned}
\tag{6.5}
$$

for which the eigenvalues read $\omega^{(PFP)}_{(\pm),\vec{k},\sigma} = -\mu \pm 2\Delta\sqrt{\cos^2(k_x) + \cos^2(k_y)}$ and are shown in figure 6.1.



(a) (b)

Figure 6.1: (a) Representation of the energy spectrum $\omega^{(PFP)}_{(-)\vec{k},\sigma} + \mu = -2\Delta\sqrt{\cos^2(k_x) + \cos^2(k_y)}$ for k_x and k_y belonging to $\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ and (b) the contour representation of the energy spectrum showing the presence of the nodal points $(\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ where the energy is equal to zero.

We are interested in the low energy behaviour of the quantum spin system described by the Hamiltonian (6.5) in the neighbourhood of the nodal points $\left(k_x = \pm\frac{\pi}{2}, \pm\frac{\pi}{2}\right)$ where the energy gap $\left(\omega^{(PFP)}_{(+),\vec{k},\sigma} - \omega^{(PFP)}_{(-),\vec{k},\sigma}\right)$ vanishes as shown in figure 6.1.

As already shown in earlier work by Ghaemi and Senthil [28] and Morinari [57] the spin liquid Hamiltonian (6.5) for spin systems at low energy can be described by four-component Dirac spinons and the corresponding Dirac Hamiltonian reads

$$
H = \sum_{\vec{k} \in SBZ} \sum_{\sigma} \psi^\dagger_{\vec{k}\sigma} \left[-\mu \mathbb{I} + \widetilde{\Delta} k_+ \begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_2 \end{pmatrix} - \widetilde{\Delta} k_- \begin{pmatrix} \tau_2 & 0 \\ 0 & \tau_1 \end{pmatrix} \right] \psi_{\vec{k}\sigma} \tag{6.6}
$$

$k_+ = k_x + k_y$ and $k_- = k_x - k_y$, $\widetilde{\Delta} = 2\Delta \cos\frac{\pi}{4}$ and

$$\psi_{\vec{k}\sigma} = \begin{pmatrix} f_{1a,\vec{k}\sigma} \\ f_{1b,\vec{k}\sigma} \\ f_{2a\vec{k}\sigma} \\ f_{2b\vec{k}\sigma} \end{pmatrix} \tag{6.7}$$

Indices 1 and 2 in the definition of ψ given by equation (6.7) refers to the two independent nodal points $\left(\frac{\pi}{2}, \frac{\pi}{2}\right)$ and $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$, indices a and b originate from a linear transformation between $f_{\vec{k}}$ and $f_{\vec{k}+\vec{\pi}}$ as detailed in appendix E.1.

The Dirac action of a spin liquid in (2+1) dimensions is derived in appendix E.1. In Euclidean space the action reads

$$S_E = \int_0^\beta d\tau \int d^2\vec{r} \sum_\sigma \bar{\psi}_{\vec{r}\sigma} \left[\gamma^0 \left(\partial_\tau - \mu\right) + \widetilde{\Delta}\gamma^k \partial_k\right] \psi_{\vec{r}\sigma} \tag{6.8}$$

where $\widetilde{\Delta} = 2\Delta \cos\frac{\pi}{4}$ is the "light velocity" space component of the three "light velocity" vector $v_\mu = \left(1, \widetilde{\Delta}, \widetilde{\Delta}\right)$, and the $\{\gamma^\mu\}$'s are the Dirac gamma matrices in (2+1) dimensions.

6.2.1 "Gravitational" effects

In the action (6.8) the "light velocity" v_μ which is affected by the parameter $\widetilde{\Delta}$ can be seen as a space-time curvature parameter. This term must modify the covariant derivative due to the "gravitational" effect induced by the "light velocity" term. We show now in which way one must modify the theory in order to include this gravitational effect which finally is no longer important in our spinon action.

In a curved space-time the Dirac action of a relativistic fermion reads [68]

$$S_{Dirac} = \int d^3x E \bar{\psi} \gamma^p e_p^\mu \left(\partial_\mu + \frac{1}{8}\omega_{\mu,ab}\left[\gamma^a, \gamma^b\right]\right)\psi \tag{6.9}$$

where e_p^μ are triads (also called *dreibein*) and $E = \det e_p^\mu$ relates the "flat" space (with "flat" index m, where there is no gravitational effect) and the curved space (with "curvy" index μ, where there is a gravitational effect). The second term in brackets (equation (6.9) , where $\omega_{\mu,ab}$ is the connection coefficient) comes from the preservation of the *local* invariance under Lorentz transformations in the presence of curved space-time [68] (it is similar to the gauge invariance transformation of the covariant derivative $\partial_\mu \to D_\mu$).

Comparing equation (6.8) with (6.9) one shifts the imaginary time derivation $\partial_\tau \to \partial_\tau + \mu$ in (6.8) which leads to a new definition of the Matsubara frequencies only for the fermion fields ψ [66]. These frequencies read

$$\widetilde{\omega}_{F,n} = \omega_{F,n} - \mu/i = \frac{2\pi}{\beta}(n + 1/4) \tag{6.10}$$

Further we define the *dreibein* as

$$e_p^\mu = \begin{pmatrix} \frac{1}{\sqrt{\widetilde{\Delta}}} & 0 & 0 \\ 0 & \sqrt{\widetilde{\Delta}} & 0 \\ 0 & 0 & \sqrt{\widetilde{\Delta}} \end{pmatrix}$$

Hence spinons move in a "gravitational" field which can be characterized by the metric

$$g_{\mu\nu} = \delta^{mn} e_m^\mu e_n^\nu = \begin{bmatrix} \frac{1}{\widetilde{\Delta}} & 0 & 0 \\ 0 & \widetilde{\Delta} & 0 \\ 0 & 0 & \widetilde{\Delta} \end{bmatrix} \tag{6.11}$$

One should add the term

$$\int_0^\beta d\tau \int d^2\vec{r} E \sum_\sigma \bar{\psi}_{\vec{r}\sigma} \gamma^p \left[e_p^\mu \frac{1}{8} \omega_{\mu,ab} \left[\gamma^a, \gamma^b\right] \right] \psi_{\vec{r}\sigma} \tag{6.12}$$

in equation (6.8) in order to verify the *local* invariance of the Lorentz transformation under the "gravitational" field. The metric can be handled [79] assuming $\widetilde{\Delta} = 1$ without altering the physics of the problem as we will explain below.

Since the metric (6.11) is no longer that of a flat space-time the connection coefficient $\omega_{\mu,ab}$ is defined by

$$\omega_{\mu,ab} = -\left(\partial_\mu e_{ab} - \Gamma_{\mu a}{}^{\gamma} e_{\gamma b}\right) \tag{6.13}$$

The Γ's are Christoffel symbols ($\Gamma_{\mu\nu\gamma} = \frac{1}{2}\left(g_{\mu\nu,\gamma} + g_{\mu\gamma,\nu} - g_{\nu\gamma,\mu}\right)$ with $g_{\mu\nu,\gamma} = \partial_\gamma g_{\mu\nu}$) and e_a^μ are the *dreibein*. Since $\widetilde{\Delta}$ can be considered as constant in space-time we see clearly that the *dreibein* are also constant with respect to the space-time coordinates. Hence $\omega_{\alpha,ab} = 0$ in a dilated flat space-time with the Euclidean metric (6.11). Since we showed that (6.12) is equal to zero one can put $\widetilde{\Delta} = 1$ in equation (6.8) and finally equation (6.8) reduces to

$$S_E = \int_0^\beta d\tau \int d^2\vec{r} \sum_\sigma \bar{\psi}_{\vec{r}\sigma}(\tau) \gamma_\mu \partial_\mu \psi_{\vec{r}\sigma}(\tau) \tag{6.14}$$

Recall that we shifted the time derivative ∂_τ by the imaginary chemical potential μ modifying the Mastubara frequencies (6.10). More details concerning the modification of the Matsubara frequencies are given in subsection 3.3.4. This modification will induce substantial consequences as it will be shown in the following.

6.2.2 Quantum Electrodynamic Spinon action in (2+1) dimensions

Since the Heisenberg Hamiltonian (6.6) is gauge invariant in the $U(1)$ transformation $\psi \rightarrow e^{ig\theta}\psi$, where θ is a space-dependent scalar function, the Dirac action can be written in the form

$$S_E = \int_0^\beta d\tau \int d^2\vec{r} \;\; \Bigg\{ \;\; -\frac{1}{2}a_\mu\left(\vec{r},\tau\right)\left[\left(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu\right)\right]a_\nu\left(\vec{r},\tau\right) \\ + \;\; \sum_\sigma \bar{\psi}_{\vec{r}\sigma}\left(\tau\right)\left[\gamma_\mu\left(\partial_\mu - iga_\mu\right)\right]\psi_{\vec{r}\sigma}\left(\tau\right)\Bigg\} \qquad (6.15)$$

Here g comes as the coupling strength between the gauge field a_μ and the Dirac spinons ψ. The gauge field a_μ is related to the phase $\theta\left(\vec{r}\right)$ of the spinon at site $\vec{r}$ through the gauge transformation $f_{\vec{r},\sigma} \rightarrow e^{ig\theta(\vec{r})}f_{\vec{r},\sigma}$ which keeps the Heisenberg Hamiltonian invariant. From the definition of ψ one gets $\psi_{\vec{r}\sigma} \rightarrow e^{ig\theta(\vec{r})}\psi_{\vec{r}\sigma}$. It is clear that $\theta\left(\vec{r}\right)$ is the phase at the lattice site $\vec{r}$ and that $a_\mu\left(\vec{r}\right) = \partial_\mu\theta\left(\vec{r}\right)$. Hence the fluctuations of the flux ϕ through the plaquette (see figure 5.2) are directly related to the circulation of the gauge field a_μ around the plaquette

$$\begin{aligned} \phi &= g\sum_{<i,j>\in\Box}\left(\theta\left(\vec{r_i}\right) - \theta\left(\vec{r_j}\right)\right) \\ &= g\int_\Box d\vec{l}.\vec{a} \end{aligned}$$

Phase fluctuations of lattice sites are measured by the gauge field a_μ. In (6.15) the first term corresponds to the "Maxwell" term $-\frac{1}{4}f_{\mu\nu}f^{\mu\nu}$ of the gauge field a_μ where $f^{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$, λ is the parameter of the Faddeev-Popov gauge fixing term $-\lambda\left(\partial^\mu a_\mu\right)^2$ [39], $\delta^{\mu\nu}$ the Kronecker δ and $\Box = \partial_\tau^2 + \vec{\nabla}^2$ is the Laplacian in Euclidean space-time.

Since the spinons ψ are minimally coupled to the gauge field a_μ, materializing the effect of fluctuations around the mean-field spin liquid ansatz described by the "Diffuson", the energy-momentum conservation leads to consider the gauge-invariant and symmetric energy-momemtum tensor

$$\Theta_{\mu\nu} = \frac{\partial\mathcal{L}}{\partial\left(\partial_\mu a_\delta\right)}\partial_\nu a_\delta - g_{\mu\nu}\mathcal{L} + \partial_\rho\left(f_{\mu\rho}a_\nu\right) \qquad (6.16)$$

where $\mathcal{L}$ is the QED_3 Lagrangian of the spinon deriving from $S_E = \int_0^\beta d\tau\mathcal{L}$ in the Euclidean space. The Maxwell Lagrangian $-\frac{1}{4}f_{\mu\nu}f^{\mu\nu} = \frac{1}{2}a_\mu\left(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu\right)a_\nu$ is added to (6.14) in order to verify the energy-momentum conservation [39]

$$\partial_\mu\Theta_{\mu\nu} = 0 \qquad (6.17)$$

Notice that "photon" described by the gauge field a_μ are not present in nature and thus the dynamical Maxwell term above looks inadequate as it stands. In order to be coherent one should do the change of variable

$$a_\mu = a_\mu/g \tag{6.18}$$

where g is the coupling constant between the spinon and the gauge field. The spinon action (6.15) reads

$$S_E = \int_0^\beta d\tau \int d^2\vec{r} \quad \left\{ \quad -\frac{1}{2g^2} a_\mu\left(\vec{r},\tau\right)\left[(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu)\right] a_\nu\left(\vec{r},\tau\right) \right.$$
$$\left. + \quad \sum_\sigma \bar{\psi}_{\vec{r}\sigma}\left(\tau\right)\left[\gamma_\mu\left(\partial_\mu - i a_\mu\right)\right]\psi_{\vec{r}\sigma}\left(\tau\right) \right\} \tag{6.19}$$

The dynamical term can now be removed in the limit of $g \to \infty$ verifying the energy-momentum conservation law (6.17). In this limit we are treating a ***strongly correlated*** electron system. Keeping this in mind we go further in the development using (6.15).

6.3 The "Photon" propagator at finite temperature

Integrating over the fermion fields ψ, using relation (A.24) in appendix A, the partition function $\mathcal{Z}\left[\psi, a\right] = \int \mathcal{D}\left(\psi, a\right) e^{-S_E}$ with action S_E given by equation (6.15) leads to the pure gauge partition function

$$\mathcal{Z}\left[a\right] = \int \mathcal{D}\left(a\right) e^{-S_{eff}[a]} \tag{6.20}$$

where the effective pure gauge field action $S_{eff}\left[a\right]$ comes in the form

$$S_{eff}\left[a\right] = \int_0^\beta d\tau \int d^2\vec{r} \left\{ -\frac{1}{2} a_\mu\left[(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu)\right] a_\nu \right\} - \ln\det\left[\gamma_\mu\left(\partial_\mu - i g a_\mu\right)\right] \tag{6.21}$$

Here one recognizes similarity between the second term in (6.21) and the *log-det* term in (4.39). Following the same steps as in section 4.4 one can develop the second term in the effective gauge field action $S_{eff}\left[a\right]$ into a series and write

$$\ln\det\left[\gamma_\mu\left(\partial_\mu - i g a_\mu\right)\right] = \ln\det G_F^{-1} - \sum_{n=1}^{\infty} \frac{1}{n} Tr\left[i G_F \gamma^\mu a_\mu\right]^n \tag{6.22}$$

where $G_F^{-1}(k-k^{'}) = i\frac{\gamma^\mu k_\mu}{(2\pi)^2\beta}\delta(k-k^{'})$ is the fermion Green function in the Fourier space-time with $k = \left(\widetilde{\omega}_{F,n}, \vec{k}\right)$, hence $G_F = -i\frac{\gamma^\mu k_\mu}{k^2}(2\pi)^2\beta\delta\left(k-k^{'}\right)$. The first term on the right hand side of equation (6.22) being independent of the gauge field $\{a_\mu\}$ can be removed from the series since we focus our attention on pure gauge field terms. The first term proportional to the gauge field $n=1$ in the sum vanish since $tr\gamma_\mu = 0$. Keeping only second order terms in the gauge field in order to treat gaussian fluctuations one gets the pure gauge action

$$\begin{aligned} S^{(2)}_{eff}\left[a\right] &= \int_0^\beta d\tau \int d^2\vec{r}\left\{-\frac{1}{2}a_\mu\left[(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu)\right]a_\nu\right\} \\ &+ g^2\frac{1}{2\beta}\sum_\sigma\sum_{\omega_{F,1}}\int\frac{d^2\vec{k}_1}{(2\pi)^2}.\frac{1}{\beta}\sum_{\omega_F^{''}}\int\frac{d^2\vec{k^{''}}}{(2\pi)^2} \\ & tr\left[\frac{\gamma^\rho k_{1,\rho}}{k_1^2}.\gamma^\mu a_\mu(k_1-k^{''}).\frac{\gamma^\eta k^{''}_\eta}{k^{''2}}.\gamma^\nu a_\nu\left(-(k_1-k^{''})\right)\right] \end{aligned} \tag{6.23}$$

The second term in equation (6.23) is worked out in details in appendix E.2 and one gets

$$S^{(2)}_{eff} = -\frac{1}{2\beta}\sum_{\omega_B}\int\frac{d^2\vec{q}}{(2\pi)^2}a_\mu(-q)\left[\Delta^{(0)^{-1}}_{\mu\nu} + \Pi_{\mu\nu}(q)\right]a_\nu(q) \tag{6.24}$$

$\Delta^{(0)^{-1}}_{\mu\nu} = [(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu)]$ is the bare photon propagator. The detailed calculation of the polarization function $\Pi_{\mu\nu}$ is given in appendix E.2. Equations (E.23) and (E.24) give the components of $\Pi_{\mu\nu}$. The finite-temperature dressed photon propagator in Euclidean space (imaginary time formulation) verifies the Dyson equation

$$\Delta^{-1}_{\mu\nu} = \Delta^{(0)^{-1}}_{\mu\nu} + \Pi_{\mu\nu} \tag{6.25}$$

Finally the gauge effective action reads $S^{(2)}_{eff} = -\frac{1}{2\beta}\sum_{\omega_B}\int\frac{d^2\vec{q}}{(2\pi)^2}a_\mu(-q)\Delta^{-1}_{\mu\nu}(q)\,a_\nu(q)$.

6.3.1 Comparison of the Popov and Fedotov procedure with the Lagrange multiplier method

Table 6.1 compares the polarization function components $\widetilde{\Pi}_1$, $\widetilde{\Pi}_2$ and $\widetilde{\Pi}_3$ obtained by means of the Lagrange multiplier approximation for which $\lambda = 0$ as shown in section 5.2 with the PFP as computed in appendix E.2. Differences appear in the denominator term $D(X,Y)$ and in the numerator of the integrant in $\widetilde{\Pi}_2$ where the cosine terms are replaced by sine terms.

We now push the comparison further and show below how the PFP modifies the effective potential between two test particles and also affects the dynamically generated mass of the spinons.

Table 6.1: Comparison of polarization function components obtained from the Lagrange multiplier approximation and the Popov and Fedotov procedure

$\alpha = 2.g^2$	Lagrange multiplier method	PFP
$\widetilde{\Pi}_1$	$\frac{\alpha q}{\pi}\int_0^1 dx\sqrt{x(1-x)}\frac{\sinh\beta q\sqrt{x(1-x)}}{D(X,Y)}$	$\frac{\alpha q}{\pi}\int_0^1 dx\sqrt{x(1-x)}\frac{\sinh\beta q\sqrt{x(1-x)}}{D(X,Y)}$
$\widetilde{\Pi}_2$	$\frac{\alpha m}{\beta}\int_0^1 dx(1-2x)\frac{\sin 2\pi xm}{D(X,Y)}$	$\frac{\alpha m}{\beta}\int_0^1 dx(1-2x)\frac{\cos 2\pi xm}{D(X,Y)}$
$\widetilde{\Pi}_3$	$\frac{\alpha}{\pi\beta}\int_0^1 dx\ln 2D(X,Y)$	$\frac{\alpha}{\pi\beta}\int_0^1 dx\ln 2D(X,Y)$
$D(X,Y)$	$\cosh\left(\beta q\sqrt{x(1-x)}\right)+\cos(2\pi xm)$	$\cosh\left(\beta q\sqrt{x(1-x)}\right)+\sin(2\pi xm)$

6.3.2 Covariant description of the polarization function

One may believe that a system at finite temperature breaks Lorentz invariance since the frame described by the heat bath already selects out a specific Lorentz frame. However this is not true and one can formulate the statistical mechanics in a Lorentz covariant form [19].

We consider the three dimensional Euclidean space. Define the proper 3-velocity u^μ of the heat bath. In the rest frame of the heat bath the three velocity has the form $u^\mu = (1,0,0)$ and the inverse temperature β characterizes the thermal property of the heat bath.

Given the 3-velocity vector u^μ one can decompose any three vector into parallel and orthogonal components with respect to the proper velocity of the heat bath, the velocity u^μ. In particular the parallel and transversal components of the three momentum q^μ with respect to u^μ read

$$q_{\|}^{\mu} = (q.u)\, u^{\mu} \tag{6.26}$$

$$\widetilde{q}^{\mu} = q^{\mu} - q_{\|}^{\mu} \tag{6.27}$$

Similarly one can decompose any vector and tensor into components which is parallel and transverse to a given momentum vector q^μ

Figure 6.2: The dressed photon propagator. Wavy lines correspond to the photon and solid loops to the fermion insertions

$$\bar{u}_\mu = u_\mu - \frac{(q.u)}{q^2} q_\mu \tag{6.28}$$

$$\bar{\eta}_{\mu\nu} = \delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \tag{6.29}$$

It is now easy to define second rank symmetric tensors $T_{\mu\nu}$ constructed at finite temperature from q^μ, u^μ and $\delta_{\mu\nu}$ which verifies $q^\mu T_{\mu\nu} = 0$

$$A_{\mu\nu} = \delta_{\mu\nu} - u^\mu u^\nu - \frac{\widetilde{q}_\mu \widetilde{q}_\nu}{\widetilde{q}^2} \tag{6.30}$$

$$B_{\mu\nu} = \frac{q^2}{\widetilde{q}^2} \bar{u}_\mu \bar{u}_\nu \tag{6.31}$$

$$C_{\mu\nu} = \delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \tag{6.32}$$

where $A_{\mu\nu}$ and $B_{\mu\nu}$ verifies the relation

$$A_{\mu\nu} + B_{\mu\nu} = C_{\mu\nu} \tag{6.33}$$

Since one considers a spin system at finite temperature and "relativistic" covariance should be preserved the polarization function may be put in the general form [19]

$$\Pi_{\mu\nu} = \Pi_A A_{\mu\nu} + \Pi_B B_{\mu\nu} \tag{6.34}$$

and the Dyson equation (6.25) can now be expressed in a covariant form if one uses relation (6.34).

6.3.3 Dressed "photon" propagator

Inverting the Dyson equation (6.25) the dressed photon propagator $\Delta_{\mu\nu}$ is obtained by summation of the geometric series

$$\Delta_{\mu\nu} = \Delta^{(0)}_{\mu\nu} + \Delta^{(0)}_{\mu\alpha}.(-\Pi^{\alpha\beta}).\Delta^{(0)}_{\beta\nu} + \Delta^{(0)}_{\mu\alpha}.(-\Pi^{\alpha\beta}).\Delta^{(0)}_{\beta\delta}.(-\Pi^{\delta\rho}).\Delta^{(0)}_{\rho\nu} + \cdots \tag{6.35}$$

Figure 6.2 shows the Feynman diagrammatic representation of the Dyson series (6.35). The dressed photon propagator reads

$$\Delta_{\mu\nu} = \frac{A_{\mu\nu}}{q^2 + \Pi_A} + \frac{B_{\mu\nu}}{q^2 + \Pi_B} - (1 - 1/\lambda)\frac{q_\mu q_\nu}{(q^2)^2} \tag{6.36}$$

where Π_A and Π_B are related to $\widetilde{\Pi}_k$ by

$$\Pi_A = \widetilde{\Pi}_1 + \widetilde{\Pi}_2 \tag{6.37}$$

$$\Pi_B = \widetilde{\Pi}_3 \tag{6.38}$$

The expressions of $\widetilde{\Pi}_1$, $\widetilde{\Pi}_2$ and $\widetilde{\Pi}_3$ are explicitly worked out in appendix E.2. Here $q^0 = \frac{2\pi}{\beta}m$ is the boson Matsubara frequency energy component of the photon three-vector q^μ.

The dressed photon propagator is clearly expressed in a covariant form since the basis tensor $A_{\mu\nu}$ and $B_{\mu\nu}$ are as shown in subsection 6.3.2. Remarkably the dressed photon propagator is composed of a longitudinal and a transverse part with respect to the photon momentum q_μ unlike the bare photon propagator ${\Delta^{(0)}_{\mu\nu}}^{-1} = \frac{1}{q^2}\left[\delta_{\mu\nu} - (1 - 1/\lambda)\,\frac{q_\mu q_\nu}{q^2}\right]$ when one takes the Landau gauge fixing condition $\lambda \to \infty$. Even $\Pi_{\mu\nu}$ is transverse to the photon momentum q_μ. In the Landau gauge one gets

$$\Delta_{\mu\nu} = \frac{A_{\mu\nu}}{q^2 + \Pi_A} + \frac{B_{\mu\nu}}{q^2 + \Pi_B} - \frac{q_\mu q_\nu}{(q^2)^2} \tag{6.39}$$

showing clearly that the dressed photon propagator presents a longitudinal part with respect to the photon momentum since $q_\mu A_{\mu\nu} = q_\mu B_{\mu\nu} = 0$.

6.3.4 Effective potential between test particles

The questions to which one answers here concern the derivation of the effective potential interacting between two spinons and the impact of PFP site-occupation constraint on it.

The spinon action (6.15) describes a gas of spinons and photons coupled together by a coupling constant g which can be interpreted as the charge of the spinon. Paying attention to the analogy with a plasma made of electrons and the spinon gas one can identify the interaction between two spinon like one would identify the interaction between two electrons. The term proportional to the product $q_a.q_b$ where q_a and q_b are the charges of particles a and b correspond to the Coulomb interaction between two charge and reads

$$V(R = |\vec{r}_a - \vec{r}_b|) = -2\pi q_a q_b \ln\left(|\vec{r}_a - \vec{r}_b|\right) \tag{6.40}$$

in a two-dimensional system where particles are at position $\vec{r}_a$ with charge q_a and $\vec{r}_b$ with charge q_b. The corresponding action comes as

$$S_{plasma} = \frac{\beta}{2}\left\{\sum_{a\neq b} - q_a q_b 2\pi \ln\left(|\vec{r}_a - \vec{r}_b|\right) + \text{const.}\sum_a q_a^2\right\} \tag{6.41}$$

for a plasma two-dimensional system at temperature $1/\beta$. Define the spinon three-current $j_\mu = -ig\sum_\sigma \bar{\psi}_\sigma \gamma_\mu \psi_\sigma$ where ψ is the Dirac spinor of the spinon defined in section 6.2. In a classical picture the time component of the current vector reads $j_0(x) = \sum_a q_a \delta(x - x_a)$. Identifying the charge q with the component j_0 of the three-vector j_μ the Coulomb interaction comes as

$$V(R) = q_a . q_b \frac{\partial^2}{\partial j_0(R,\tau)\,\partial j_0(0,\tau)} \ln \mathcal{Z} \tag{6.42}$$

where $\mathcal{Z} \propto e^{-S_{plasma}}$ is the partition function of the corresponding action S_{plasma}. Now using relation (6.42) with the partition function $\mathcal{Z}[\psi, a] = \int \mathcal{D}(\psi, a)\, e^{-S_E}$ with the spinon action S_E given by equation (6.15) and rewritten as

$$\begin{aligned} S_E = \int_0^\beta d\tau \int d^2\vec{r} \quad \Big\{ & \quad -\frac{1}{2} a_\mu(\vec{r},\tau)\left[(\Box\delta^{\mu\nu} + (1-\lambda)\partial^\mu\partial^\nu)\right] a_\nu(\vec{r},\tau) \\ + & \quad \sum_\sigma \bar{\psi}_{\vec{r}\sigma}(\tau)\,\gamma_\mu\partial_\mu\psi_{\vec{r}\sigma}(\tau) + j_\mu(\vec{r},\tau)\, a_\mu(\vec{r},\tau) \Big\} \end{aligned} \tag{6.43}$$

Considering the term proportional in j_μ, one finally gets from deriving the effective potential

$$V(R) = q_a q_b \int_0^\beta d\tau < a_0(R,\tau)\, a_0(0,\tau) > \tag{6.44}$$

Here $< a_0(R,\tau)\, a_0(0,\tau) >$ is to identify with the dressed photon propagator time components Δ_{00}. The effective static potential $V(R)$ between two test particles (spinons) of opposite chages $q_a = -q_b = g$ at distance R is given by

$$V(R) \quad = \quad -g^2 \int_0^\beta d\tau \Delta_{00}(\tau, R) \tag{6.45}$$

After a Fourier transformation on Δ_{00} the time components of the dressed propagator $\Delta_{\mu\nu}$ in equation (6.45) one gets

$$V(R) = -g^2 \frac{1}{2\pi} \int \frac{d^2\vec{q}}{(2\pi)^2} \Delta_{00}(q^0 = 0, \vec{q}) e^{i\vec{q}.\vec{R}} \tag{6.46}$$

with

$$\Delta_{00}\left(q^0 = 0, \vec{q}\right) = \frac{1}{q^2 + \widetilde{\Pi}_3\left(q^0 = \frac{2\pi}{\beta} m = 0\right)} \tag{6.47}$$

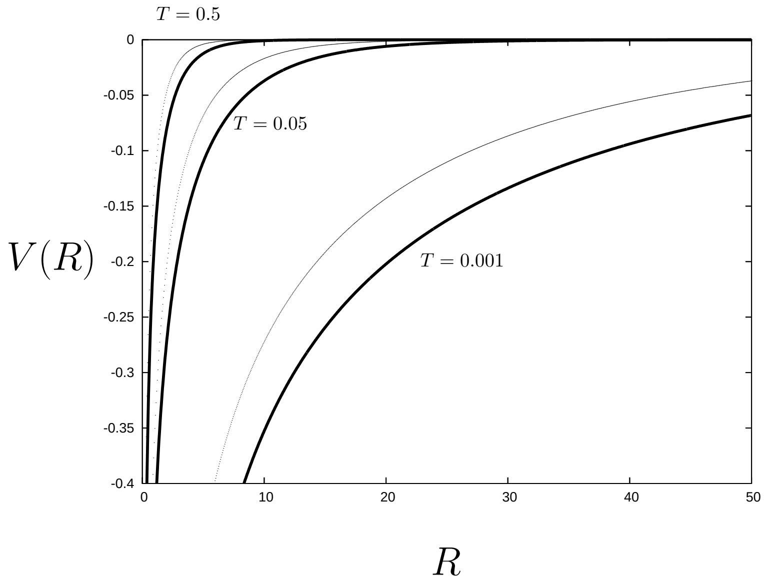


Figure 6.3: Effective static potential with (fat line) and without (dotted line) the Popov-Fedotov imaginary chemical potential for the temperature $T = \{0.001, 0.05, 0.5\}$.

The effective potential then reads

$$V(R) = -\frac{g^2}{2\pi}\int_0^\infty dqqJ_0(qR).\frac{1}{q^2 + \widetilde{\Pi}_3(m=0)} \tag{6.48}$$

where $J_0(qR)$ is the zero order Bessel function of the first kind.

The polarization contribution $\widetilde{\Pi}_3(q^0 = 0, \vec{q})$ is equal to $\frac{\alpha}{\pi\beta}\int_0^1 dx \ln\left(2\cosh\beta q\sqrt{x(1-x)}\right)$ when taking the Popov and Fedotov imaginary chemical potential into account. This has to be compared to the expression $\frac{2\alpha}{\pi\beta}\int_0^1 dx \ln\left(2\cosh\frac{\beta}{2}q\sqrt{x(1-x)}\right)$ when the Lagrange multiplier method for which $\lambda = 0$ is used [24], a detailed comparaison is given in table 6.1.

For small momentum $q \to 0$, $\widetilde{\Pi}_3(m=0)$ can be identified as a mass term $(M_0^{(PFP)}(\beta))^2$ and reads

$$\lim_{q\to 0}\widetilde{\Pi}_3(m=0) = (M_0^{(PFP)}(\beta))^2 = \frac{\alpha}{\pi\beta}\ln 2 \tag{6.49}$$

For $R \gg (M_0^{(PFP)})^{-1}$ the effective potential reads

$$\begin{aligned} V(R,\beta) &\simeq -\frac{g^2}{2\pi}\int_0^\infty dq\frac{qJ_0(qR)}{q^2 + \left(M_0^{(PFP)}\right)^2} \\ &= -\frac{\alpha}{N}\sqrt{\frac{1}{8\pi RM_0^{(PFP)}}}e^{-M_0^{(PFP)}R} \end{aligned}$$

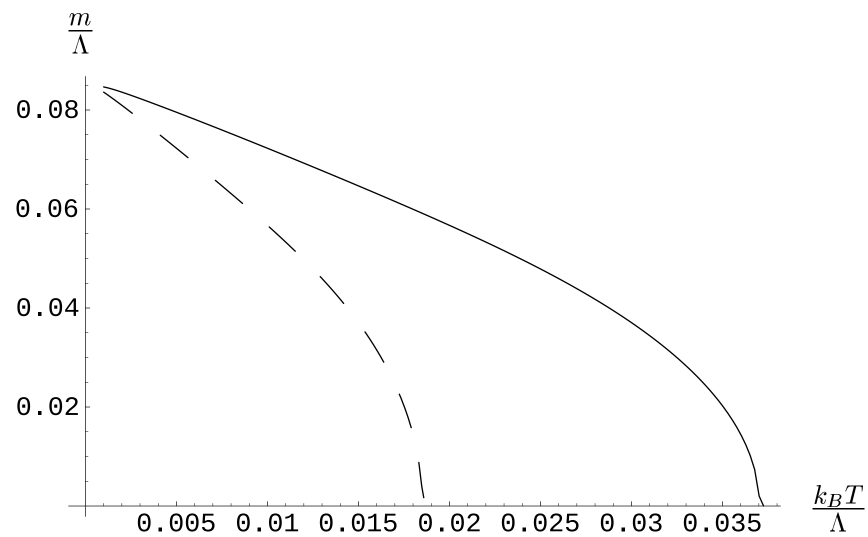


Figure 6.4: Temperature dependence of the dynamical mass generated with (full line) and without (dashed line) the use of the Popov-Fedotov procedure.

where $N = 2$ since we consider only $S = 1/2$ spins.

Figure 6.3 shows the effective potential between two opposite test charges at distance $R \gg (M_0^{(PFP)})^{-1}$. The screening effect is smaller when the imaginary PFP chemical potential μ is implemented rather than the Lagrange multiplier λ. By inspection one sees that $(M_0^{(PFP)})^{-1} = \sqrt{2}(M_0^{(\lambda)})^{-1}$. The main effect of combinating of the PFP and thermal fluctuations is to increase the range of effective static interaction, which is infinite at zero temperature, between two test particles of opposite charges compared to the case where the Lagrange multiplier method is used.

6.4 Dynamical mass generation

Appelquist et al. [5, 6] have shown that at zero temperature the originally massless fermion can acquire a dynamically generated mass when the number N of fermion flavors is lower than the critical value $N_c = 32/\pi^2$. Later Maris [52] confirmed the existence of a critical value $N_c \simeq 3.3$ below which a dynamical mass can be generated. Since we consider only spin-1/2 systems, $N = 2$ and hence $N < N_c$.

At finite temperature Dorey and Mavromatos [24] and Lee [48] have shown that the dynamically generated mass vanishes at a temperature T larger than the critical one T_c.

We now show how the Popov and Fedotov procedure doubles the "chiral" restoring transition temperature T_c of the dynamical mass generation. The Schwinger-Dyson equation for the spinon propagator at finite temperature reads

$$G^{-1}(k) = G^{(0)^{-1}}(k) - \frac{g}{\beta}\sum_{\widetilde{\omega}_{F,n}} \int \frac{d^2\vec{P}}{(2\pi)^2}\gamma_\mu G(p)\Delta_{\mu\nu}(k-p)\Gamma_\nu \tag{6.50}$$

where $p = (p_0 = \widetilde{\omega}_{F,n}, \vec{P})$, G is the spinon propagator, Γ_ν the spinon-"photon" vertex which will be approximated here by its bare value $g\gamma_\nu$ and $\Delta_{\mu\nu}$ the dressed photon propagator (6.36). The second term in (6.50) is the fermion self-energy Σ, $(G^{-1} = G^{(}0)^{-1} - \Sigma)$. Performing the trace over the γ matrices in equation (6.50) leads to a self-consistent equation for the self-energy

$$\Sigma(k) = \frac{g^2}{\beta} \sum_{\widetilde{\omega}_{F,n}} \int \frac{d^2\vec{P}}{(2\pi)^2} \Delta_{\mu\mu}(k-p) \frac{\Sigma(p)}{p^2 + \Sigma(p)^2} \tag{6.51}$$

$\Sigma(k)$ corresponds to a mass term which can be estimated at low energy and momentum limit $m(\beta) = \Sigma(k) \simeq \Sigma(0)$. In this regime equation (6.51) simplifies to

$$1 = \frac{g^2}{\beta} \sum_{\widetilde{\omega}_{F,n}} \int \frac{d^2\vec{P}}{(2\pi)^2} \Delta_{\mu\mu}(-p) . \frac{1}{p^2 + m(\beta)^2} \tag{6.52}$$

Admitting that the main contribution to (6.52) comes from the longitudinal part $\Delta_{00}(0, -\vec{P})$ of the photon propagator (6.52) goes over to

$$1 = \frac{g^2}{\beta} \sum_{\widetilde{\omega}_{F,n}} \int \frac{d^2\vec{P}}{(2\pi)^2} \left(\frac{1}{\vec{P}^2 + \widetilde{\Pi}_3(m=0)} . \frac{1}{\widetilde{\omega}_{F,n}^2 + \vec{P}^2 + m(\beta)^2} \right) \tag{6.53}$$

Performing the summation over the fermion Matsubara frequencies $\widetilde{\omega}_{F,n}$ the self-consistent equation takes the form

$$1 = \frac{\alpha}{4\pi N} \int_0^\infty dP \left(\frac{P \tanh \beta \sqrt{\vec{P}^2 + m(\beta)^2}}{\left[\vec{P}^2 + \widetilde{\Pi}_3(m=0)\right] \sqrt{\vec{P}^2 + m(\beta)^2}} \right) \tag{6.54}$$

Relation (6.54) can be solved numerically with a cutoff Λ to control the ultraviolet integration limit

$$1 = \frac{\alpha}{4\pi N} \int_0^\Lambda dP \left(\frac{P \tanh \beta \sqrt{\vec{P}^2 + m(\beta)^2}}{\left[\vec{P}^2 + \widetilde{\Pi}_3(m=0)\right] \sqrt{\vec{P}^2 + m(\beta)^2}} \right) \tag{6.55}$$

It has been shown elsewhere [3] and [24] that in the limit of Λ going to ∞ numerical results are stable and finite. Figure 6.4 compares the temperature dependence of the dynamical mass generated with and without the imaginary chemical potential introduced by the Popov and Fedotov procedure where $\alpha/\Lambda = 10^5$. By inspection of equation (6.54) and the corresponding result obtained by Dorey and Mavromatos [24] and Lee [48] one sees that the imaginary chemical potential used which fixes rigorously one spin per lattice site of the original Hamiltonian (5.31) doubles the transition temperature. This result is coherent with the results obtained elsewhere [22] and shown in section 5.2 where spinons are massless.

Since the mass can be related to the spinon energy gap and $m\,(T=0)$ corresponds to the spinon-antispinon condensate $<\bar{\psi}_{\vec{k}=\vec{0}\sigma}\psi_{\vec{k}=\vec{0},\sigma}>$ an amount of energy at least equal to $m(T)$ is necessary in order to break a pair of spinon-antispinon and liberate a spinon. Interpreting the spinon as the spin excitation part breaking a Cooper pair one can identify $m(T)$ with a superconducting gap and evaluate the reduced energy gap parameter $r = \frac{2m(0)}{k_B T_c}$ where $m(0)$ is the mass at zero temperature and T_c the transition temperature for which the mass becomes zero. Dorey and Mavromatos [24] obtained $r \simeq 10$ Lee [48] computed the mass by taking into account the frequency dependence of the photon propagator and obtained $r \simeq 6$. We have shown above that the imaginary chemical potential doubles the transition temperature so that the parameter r is $\simeq 4.8$ for $\alpha/\Lambda = \infty$ to be compared with the result of Dorey and Mavromatos and $r \simeq 3$ to be compared with Lee's result. Recall that the BCS parameter r is roughly equal to 3.5 and the $YBaCuO$ parameter $r \simeq 8$ as given by the experiment [72].

6.4.1 Antiferromagnetic Néel order parameter

There is another possible physical interpretation of the dynamical generated mass different from the former one [3, 24, 48]. One may also consider it as the antiferromagnetic Néel order parameter as will be explained belove [28, 41, 57, 62].

Consider the mean-field Hamiltonian for which one takes into account both the diffuson (5.38) and the Néel ansatz (5.10). This mean-field Hamiltonian reads

$$\begin{aligned}\mathcal{H}_{MF} &= -\frac{1}{2}\sum_{i,j}\left(J^{-1}\right)_{ij}\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right).\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) + \sum_i \vec{\bar{\varphi}}_i.\vec{S}_i \\ &+ \frac{2}{|J|}\sum_{<ij>}\bar{\Delta}^{MF}_{ij}.\Delta^{MF}_{ij} + \sum_{<ij>}\left[\bar{\Delta}^{MF}_{ij}\mathcal{D}_{ij} + \Delta^{MF}_{ij}\mathcal{D}^{\dagger}_{ij}\right] - \mu N \end{aligned} \tag{6.56}$$

Following sections 6.2 and 5.1 and after some transformation steps on (6.56) one gets the Dirac action [57]

$$S_E = \int_0^\beta d\tau \int d^2\vec{r} \sum_\sigma \bar{\psi}_{\vec{r}\sigma}\left[\gamma^0\left(\partial_\tau - \mu\right) + \widetilde{\Delta}\gamma^k\partial_k - i\vec{m}_{\text{Néel}}\vec{\sigma}\right]\psi_{\vec{r}\sigma} \tag{6.57}$$

The "mass" term $\vec{m}_{\text{Néel}} \propto \vec{\bar{\varphi}}$ is similar to the dynamical generated mass $m(\beta)$ introduced above but not equal to $m(\beta)$. The Néel ansatz introduces the Pauli matrix $\vec{\sigma}$ affected to the mass term $\vec{m}_{\text{Néel}}.\vec{\sigma}$ of the spinons. In the context of the insulator compound described by the Hamiltonian (5.31) the "chiral" symmetry breaking term $\vec{m}_{\text{Néel}}.\vec{\sigma}$ corresponds to the development of Néel order [41, 62] as can be understood by simple comparison of (6.15) with (6.57). One sees that adding the Néel anstaz, pictured by the term $\vec{\bar{\varphi}}_i.\vec{S}_i$ in (6.56), changes (6.15) into (6.57) thus $\vec{m}_{\text{Néel}}$ is clearly related to the Néel order parameter.

As a consequence of this derivation the dynamical mass generation introduces naturally the concept of second order transition from a Néel phase to a genuine paramagnetic spin liquid in two dimensional quantum antiferromagnets contrary to general wisdom, as explained in [27, 28]. This general wisdom claimed that a phase transition can only take place on one hand between collinear magnets and **V**alence **B**ond **S**olid (**VBS**) paramagnets and on the other hand between non-collinear magnets and spin liquids.

Finally one can interpret the dynamically generated mass $m(\beta)$ obtained in section 6.4 as the emergence of something like a Néel phase from a spinon gas describing the spin liquid state, more precisely from a π-flux state. One may push further and say that if this interpretation is correct then one confirms the results obtained in section 5.1 and in [9, 22] concerning the doubling of the Néel order transition temperature T_c. Indeed the dynamical generated mass sees its transition temperature doubled by the PFP compared to the Lagrange multiplier method like for the Néel order parameter as shown in chapter 5.

6.5 The PFP and the confinement problem : outlook

The QED_3 theory described above deals with *noncompact* “Maxwell” theory, in other words the integration over the gauge field a_μ goes within the limits $]-\infty, \infty[$ and the Maxwell action can be described on a lattice by

$$S_{noncompact} = \frac{1}{4}\sum_{x,\mu\nu} f_{x,\mu\nu}^2 \tag{6.58}$$

In a rigorous derivation on the lattice the “Maxwell” action is in the *compact* form [65]

$$S_{compact} = \frac{1}{2}\sum_{x,\mu\nu} \left(1 - \cos f_{x,\mu\nu}\right) \tag{6.59}$$

with $f_{x,\mu\nu} = a_{x,\mu} + a_{x+\mu,\nu} - a_{x+\nu,\mu} - a_{x,\nu}$ and $-\pi \leq a_{x,\mu} \leq \pi$. Using this compact version of the Maxwell theory the partition function reads

$$\mathcal{Z} = \sum_{\{n_{x,\mu\nu}\}} \int_{-\pi}^{\pi} \prod_{x,\mu} da_{x,\mu} e^{-\frac{1}{4}\sum\limits_{x,\mu\nu}(f_{x,\mu\nu} - 2\pi n_{x,\mu\nu})^2} \tag{6.60}$$

and takes the periodicity of the action into account. $n_{x,\mu\nu}$ is an integer coming from the periodicity of the cosine and introduces new entities called instantons. Polyakov showed [65] that the compactness causes important changes in physical properties. Indeed a pure compact Maxwell theory confines test charged particles in (2+1) dimensions due to the formation of an gas of instantons. The electrostatic potential between two test particles behaves like $V(R) \propto R$ at zero temperature and (2+1) dimensions while the electrostatic potential is deconfining in the non-compact form and behaves like $V(R) \propto \ln R$ at zero temperature and in (2+1) dimensions.

However when matter fields are taken into account the system may show a deconfined phase even in the compact formulation of the theory [62]. One may ask now whether spinons deconfine or not ? A large amount of work has been devoted these last decades to the search of an answer [16, 32, 33, 41, 44, 45, 62]. The possible existence of a confinement-deconfinement transition could leads to an explanation for spin-charge separation in strongly correlated electronic systems [60]. In the present context one may ask how the Popov and Fedotov procedure affects a *compact* QED_3 theory of spinons. As seen in chapters 4 -6 previous work has shown that the PFP probably modifies the physical behaviour in a quantitative way but does not produce a deep qualitative modification. These questions are potentially open for further work.

Previous works showed that deconfined spinons (minimally coupled with a compact $U(1)$ gauge field) can appear in the region of "*a second order quantum phase transition from a collinear Néel phase to a paramagnetic spin liquid in two dimensional square lattices with quantum antiferromagnets and short ranged interactions*" [28, 75]. In this case the Hamiltonian is the one we used in our previous description with "diffusons" to which we add the term $\frac{1}{g} \sum_{<i,j> \in N.N.} \vec{S}_i.\vec{S}_j$ where g is a parameter which controls the importance of the antiferromagnetic ordering. When $g \to \infty$ we reach the algebraic spin liquid phase and when $g \to 0$ one gets the Néel phase. There is a critical coupling parameter g_c under which the spinons are gapped, condense and are confined (through a Higgs mechanism). This corresponds to the Néel phase. For g larger than g_c spinons are again confined but this time due to proliferation of instantons [73]. However these results are obtained for zero temperature and experiments have not yet proven the existence of spinons.

6.6 Summary and conclusions

We mapped a Heisenberg $2d$ Hamiltonian describing an antiferromagnetic quantum spin system onto a $QED_{(2+1)}$ Lagrangian coupling a Dirac spinon field with a $U(1)$ gauge field. In this framework we showed that the implementation of the constraint which fixes rigorously the site occupation in a quantum spin system described by a $2d$ Heisenberg model leads to a substantial quantitative modification of the transition temperature at which the dynamically generated mass vanishes in the $QED_{(2+1)}$ description. It modifies consequently the effective static potential which acts between two test particles of opposite charges [23].

The imaginary chemical potential [66] reduces the screening of this static potential between test fermions when compared to the potential obtained from standard $QED_{(2+1)}$ calculations by Dorey and Mavromatos [24] who implicitly used a Lagrange multiplier procedure in order to fix the number of particles per lattice site [7, 51] since $\lambda = 0$ at the mean-field level.

We showed that the transition temperature to “chiral” symmetry restoration corresponding to the vanishing of the spinon mass $m(\beta)$ is doubled by the introduction of the Popov-Fedotov imaginary chemical potential. The trend is consistent with earlier results concerning the value of T_c [22]. It reduces sizably the parameter $r = \frac{2m(0)}{k_B T_c}$ determined by Dorey and Mavromatos [24] and Lee [48].

Marston [53] showed that in order to remove “forbidden” $U(1)$ gauge configuration of the antiferromagnet Heisenberg model a Chern-Simons term should be naturally included in the QED_3 action and fix the total flux through a plaquette. When the magnetic flux through a plaquette is fixed the system becomes 2π-invariant in the gauge field a_μ and instantons appear in the system. This is the case when the present non-compact formulation of QED_3 is replaced by its correct compact version [64, 65].

The implementation of a Chern-Simons term [25] in a non-compact formulation of the spinon system constrained by a rigorous site occupation has been submitted to publication [20].

Chapter 7

Conclusions and outlook

There is a general consensus on the phase diagram of high-T_c superconductivity. The simplest model which seems to take account of the strong correlation physics of the high-T_c superconductors is the Hubbard model and its strong coupling limit the $t-J$ model. The schematic phase diagram of high-T_c superconductors shows an insulating antiferromagnetic phase in the underdoped regime and is well described by Heisenberg-like models. A superconducting phase is present for low temperature and for a finite range of doping with holes (or electrons) as shown in figure 2.1. Anderson presented the viewpoint of the existence of a spin liquid state for a possible key to understand the physics of highly correlated superconducting phase [4]. The concept of **R**esonating **V**alence **B**ond (**RVB**) states was further developed [43, 58] and gave rise to the notion of spin-charge separation. The inclusion of fluctuations around the corresponding "diffuson" mean-field led to a $U(1)$ gauge theory [23, 28, 50, 57] which can be treated at the one-loop level.

One of the approaches to high-T_c supercontuctivity phenomena consists in a slight doping of the superconductor materials starting from the undoped insulating antiferromagnet phase to the underdoped regime. The underdoped superconducting should retain part of the correlation features of the insulating phase. For this reason it is of high interest to study two dimensional antiferromagnetic strongly correlated spin systems.

In chapter 4 we presented and discussed applications of the mean-field and loop expansion to the determination of physical properties of antiferromagnetic Heisenberg-type systems (supraconductors in the antiferromagnet insulating phase) in spatial dimension D [21].

We worked out the expression of physical observables (magnetization and susceptibility) starting from a specific mean-field ansatz and including contributions up to first order in a loop expansion in order to investigate the effects of fluctuation corrections to mean-field contributions at the gaussian approximation. The mean-field was chosen as a Néel state which is an *a priori* reasonable choice for spin systems described in terms of unfrustrated bipartite Heisenberg model. The results were compared to those obtained in the framework of spin wave theory.

The number of particles per spin lattice site was fixed by means of the rigorous constraint imposed by the imaginary chemical potential introduced by Popov and Fedotov [66].

At low temperature the magnetization and the magnetic susceptibility are close to the spin wave value as expected, also in agreement with former work [9].

At higher temperature the fluctuation contributions of quantum and thermal nature grow to a singularity in the neighbourhood of the critical temperature. In addition the Néel order breaks $SU(2)$ symmetry of the Heisenberg Hamiltonian inducing low momentum fluctuations near T_c which is not the case in the XXZ-model.

The influence of fluctuations decreases with the dimension D of the system due to the expected fact that the mean-field contribution increases relatively to the loop contribution.

In dimension $D = 2$ the magnetization verifies the Mermin and Wagner theorem [55] for $T \neq 0$, the fluctuations are larger than the mean-field contribution for any temperature. In a more realistic description another mean-field ansatz may be necessary in order to describe the correct physics. Ghaemi and Senthil [28] introduced a specific model in which a second order phase transition from a Néel mean-field to an ASL (algebraic spin liquid) may be at work depending on the strength of interaction parameter which enters the Hamiltonian of the system. These considerations enforce the belief that another mean-field solution like ASL may be a better starting point than a Néel state when the temperature T increases.

In chapter 5 we worked out a rigorous versus average treatment of the occupation constraint on spin systems governed by Heisenberg-type Hamiltonians at the mean-field level, for different types of spin mean-field ansatz.

We showed that a strict constraint on the site occupation of a lattice quantum spin system described by Heisenberg-type models shows a sizable quantitative different localization of the critical temperature when compared with the outcome of an average occupation constraint. With an exact site-occupation by spin the transition temperature of antiferromagnetic Néel and spin liquid states order parameters are twice as large as the critical temperature one gets from an average Lagrange multiplier procedure.

The exact occupation procedure cannot be applied to a so called cooperon state mean-field Hamiltonian. Cooperons are BCS-like pairs of particles. In this scheme the number of particles is not conserved, hence it is incompatible with a strict site occupation constraint.

In a further step we mapped a Heisenberg $2d$ Hamiltonian describing an antiferromagnetic quantum spin system onto a $QED_{(2+1)}$ Lagrangian which couples a Dirac spinon field to a $U(1)$ gauge field. We considered the π-flux state approach introduced by Affleck and Marston [2, 54]. We implemented the strict site-occupation by means of the constraint imposed through Popov and Fedotov's imaginary chemical potential [66] for $SU(2)$ and used the modified Matsubara frequencies. In this framework we showed that the implementation of the PFP constraint which fixes rigorously the site occupation in a quantum spin system described by a $2d$ Heisenberg model leads to a substantial quantitative modification of the transition temperature at which the dynamically generated mass vanishes in the $QED_{(2+1)}$ description. It modifies consequently the effective static potential which acts between two test spinons of opposite coupling charge g.

The imaginary chemical potential [66] reduces the screening of the static potential between test fermions when compared to the potential obtained from standard $QED_{(2+1)}$ calculations by Dorey and Mavromatos [24].

We showed that the transition temperature corresponding to the vanishing of the spinon mass $m(\beta)$ is doubled by the introduction of the PFP. The trend is consistent with earlier results concerning the value of T_c [22]. It reduces sizably the ratio $r = \frac{2m(0)}{k_B T_c}$ between the superconducting gap $m(0)$ and the transition temperature T_c determined by Dorey and Mavromatos [24] and Lee [48].

We conclude from this work that the Popov and Fedotov procedure which treats exactly the constraint of strict site-occupation does not modify qualitatively but quantitatively the physical results obtained by means of the average Lagrange multiplier method.

The QED_3 theory described in chapter 6 deals with a non-compact version of the Abelian gauge field action. In order to remove "forbidden" $U(1)$ gauge configuration of the antiferromagnet Heisenberg model a Chern-Simons term should be naturally included in the QED_3 action [53, 20].

The compact Maxwell theory confines test charged particles in (2+1) dimensions due to the formation of an instanton gas [65]. When matter fields are taken into account the system may show a confinement/deconfinement transition [62]. The possible existence of a confinement-deconfinement transition could give an explanation for spin-charge separation in strongly correlated electronic systems [60]. The fundamental question concerning confinement invalidating a loop expansion is up to now unsettled [33, 62].

It would be interesting to implement a Chern-Simons term [25, 20] in a *compact* $U(1)$ gauge formulation of the spinon system constrained by a strict site-occupation imposed by the Popov and Fedotov procedure.

Appendix A

Grassmann algebra and coherent states

Here we review the *Grassmann* algebra and some properties of coherent states.

- The anticommutation relation of the fermion creation and annihilation operators are

$$\left\{f_\alpha, f_\beta^\dagger\right\} = \delta_{\alpha\beta} \tag{A.1}$$
$$\{f_\alpha, f_\beta\} = 0 \tag{A.2}$$
$$\left\{f_\alpha^\dagger, f_\beta^\dagger\right\} = 0 \tag{A.3}$$

- The anticommutation relations of the *Grassmann* variables with themselves and the creation and annihilation fermionic operators are

$$\begin{aligned}
\{\xi_\alpha, \xi_\lambda\} = \xi_\alpha\xi_\lambda + \xi_\lambda\xi_\alpha &= 0 && \text{(A.4)}\\
\{\xi_\alpha^*, \xi_\lambda^*\} &= 0 && \text{(A.5)}\\
\{\xi_\alpha, \xi_\lambda^*\} &= 0 && \text{(A.6)}\\
(\lambda\xi_\alpha)^* &= \lambda^*\xi_\alpha^*,\ \lambda \text{ is a complex number} && \text{(A.7)}\\
\{\xi_\alpha, f_\beta\} = \{\xi_\alpha, f_\beta^\dagger\} &= \{\xi_\alpha^*, f_\beta\} = \{\xi_\alpha^*, f_\beta^\dagger\} = 0 && \text{(A.8)}
\end{aligned}$$

where ξ^* is the conjugate of ξ_α. Consequently the product of two identical *Grassmann* variables is zero due to the anticommutation property

$$\xi_\alpha^2 = (\xi_\alpha^*)^2 = 0 \tag{A.9}$$

- Conjugation rules :

$$
\begin{aligned}
(\xi_\alpha)^* &= \xi_\alpha^* && \text{(A.10)}\\
(\xi_\alpha^*)^* &= \xi_\alpha && \text{(A.11)}
\end{aligned}
$$

Hermitic conjugation :

$$
(\xi f)^\dagger = f^\dagger \xi^* \tag{A.12}
$$

- Derivation :

$$
\begin{aligned}
\frac{\partial}{\partial \xi}(\xi^*\xi) &= \frac{\partial}{\partial \xi}(-\xi\xi^*)\\
&= -\xi^* && \text{(A.13)}
\end{aligned}
$$

Define the operator $\mathcal{O}$

$$
\mathcal{O}(\xi,\xi^*) = \alpha + \beta\xi + \gamma\xi^* + \lambda\xi^*\xi \tag{A.14}
$$

where $\alpha, \beta, \gamma, \lambda$ are complex number. With this definition

$$
\begin{aligned}
\frac{\partial}{\partial \xi}\mathcal{O}(\xi,\xi^*) &= \beta - \lambda\xi^* && \text{(A.15)}\\
\frac{\partial}{\partial \xi^*}\mathcal{O}(\xi,\xi^*) &= \gamma + \lambda\xi && \text{(A.16)}\\
\frac{\partial}{\partial \xi}\frac{\partial}{\partial \xi^*}\mathcal{O}(\xi,\xi^*) &= \lambda\\
&= -\frac{\partial}{\partial \xi^*}\frac{\partial}{\partial \xi}\mathcal{O}(\xi,\xi^*) && \text{(A.17)}
\end{aligned}
$$

- Integration :

$$
\begin{aligned}
\int d\xi\, 1 &= \int d\xi^*\, 1 = 0 && \text{(A.18)}\\
\int d\xi\, \xi &= \int d\xi^*\, \xi^* = 1 && \text{(A.19)}
\end{aligned}
$$

Using the definition (A.14) of the operator $\mathcal{O}$

$$
\begin{aligned}
\int d\xi \mathcal{O}(\xi, \xi^*) &= \beta - \lambda \xi^* && \text{(A.20)} \\
\int d\xi^* \mathcal{O}(\xi, \xi^*) &= \gamma + \lambda && \text{(A.21)} \\
\int d\xi^* d\xi \mathcal{O}(\xi, \xi^*) &= -\lambda \\
&= -\int d\xi d\xi^* \mathcal{O}(\xi, \xi^*) && \text{(A.22)}
\end{aligned}
$$

Notice that the integration operator is equivalent to an ordinary derivation operator.

- Gaussian integrals :

  For commuting variables

$$
\int \prod_{\alpha} \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum\limits_{\alpha,\lambda} \phi_\alpha^* M_{\alpha,\lambda} \phi_\lambda + \sum\limits_{\alpha} (z_\alpha^* \phi_\alpha + z_i \phi_\alpha^*)} = [\det M]^{-\frac{1}{2}} e^{\sum\limits_{\alpha,\lambda} z_\alpha^* M_{\alpha,\lambda}^{-1} z_\lambda} \tag{A.23}
$$

  For Grassmann variables

$$
\int \prod_{\alpha} d\xi_\alpha^* d\xi_\alpha e^{-\sum\limits_{\alpha,\lambda} \xi_\alpha^* M_{\alpha,\lambda} \xi_\lambda + \sum\limits_{\alpha} (\eta_\alpha^* \xi_\alpha + \eta_\alpha \xi_\alpha^*)} = [\det M] \, e^{\sum\limits_{\alpha,\lambda} \eta_\alpha^* M_{\alpha,\lambda}^{-1} \eta_\lambda} \tag{A.24}
$$

- Coherent states :

  The fermionic coherent states $|\xi>$ are defined as

$$
\begin{aligned}
|\xi> &= e^{-\sum_\alpha \xi f_\alpha^\dagger} |0> && \text{(A.25)} \\
<\xi| &= <0| e^{\sum_\alpha \xi^* f_\alpha} && \text{(A.26)}
\end{aligned}
$$

Application of the creation and annihilation operator on coherent states leads to the following expressions

$$
\begin{aligned}
f_\alpha|\xi> &= \xi_\alpha|\xi> && \text{(A.27)}\\
f_\alpha^\dagger|\xi> &= f_\alpha^\dagger\prod_\lambda\left(1-\xi_\lambda f_\lambda^\dagger\right)|0> \\
&= f_\alpha^\dagger\left(1-\xi_\alpha f_\alpha^\dagger\right)\prod_{\lambda\neq\alpha}\left(1-\xi_\lambda f_\lambda^\dagger\right)|0> \\
&= \left(f_\alpha^\dagger\right)\prod_{\lambda\neq\alpha}\left(1-\xi_\lambda f_\lambda^\dagger\right)|0> \\
&= -\frac{\partial}{\partial\xi_\alpha}\left(1-\xi_\alpha f_\alpha^\dagger\right)\prod_{\lambda\neq\alpha}\left(1-\xi_\lambda f_\lambda^\dagger\right)|0> \\
&= -\frac{\partial}{\partial\xi_\alpha}|\xi> && \text{(A.28)}\\
<\xi|f_\alpha &= \frac{\partial}{\partial\xi^*}<\xi| && \text{(A.29)}\\
<\xi|f_\alpha^\dagger &= <\xi|\xi_\alpha^* && \text{(A.30)}
\end{aligned}
$$

The *overlap* of two coherent states is

$$
\begin{aligned}
<\xi|\xi^{'}> &= <0|\prod_\alpha(1+\xi_\alpha^* f_\alpha)(1-\xi_\alpha^{'} f_\alpha^\dagger)|0> && \text{(A.31)}\\
&= e^{\sum_\alpha \xi^*\xi^{'}} && \text{(A.32)}
\end{aligned}
$$

and the elements of fermionic operators between two different coherent states $|\xi>$ and $|\xi^{'}>$ read

$$
<\xi|\mathcal{O}\left(\{f_\alpha\},\{f_\alpha^\dagger\}\right)|\xi^{'}>=e^{\sum_\alpha \xi^*\xi^{'}}\mathcal{O}\left(\{\xi_\alpha\},\{\xi_\alpha^\dagger\}\right) \tag{A.33}
$$

Appendix B

Spin Brillouin Zone

B.1 Two dimensional bipartite lattices

Here we construct the Spin Brillouin Zone (SPZ) of a two dimensional lattice. We define the components of the wave vector $\vec{k}$ on the orthonormal reciprocal sublattice basis $\left(\vec{\tilde{e}}_1, \vec{\tilde{e}}_2\right)$ which is given by $\vec{\tilde{e}}_i . \vec{e}_j = \delta_{ij}$ where the direct basis is defined as

$$\vec{e}_1 = \frac{1}{\sqrt{2}} \left(\vec{e}_x + \vec{e}_y\right) \tag{B.1}$$

$$\vec{e}_2 = \frac{1}{\sqrt{2}} \left(\vec{e}_x - \vec{e}_y\right) \tag{B.2}$$

Since the direct basis is already orthonormal the reciprocal basis is identically equal to the first one $\left(\vec{\tilde{e}}_1 = \vec{e}_1, \vec{\tilde{e}}_2 = \vec{e}_2\right)$. Figure B.1 shows a two dimensional bipartite lattice where blue points refers to one type A and red points to an other type B of sublattices. The crystal basis $(\vec{e}_x, \vec{e}_y)$ as well as the direct basis $(\vec{e}_1, \vec{e}_2)$ are shown.

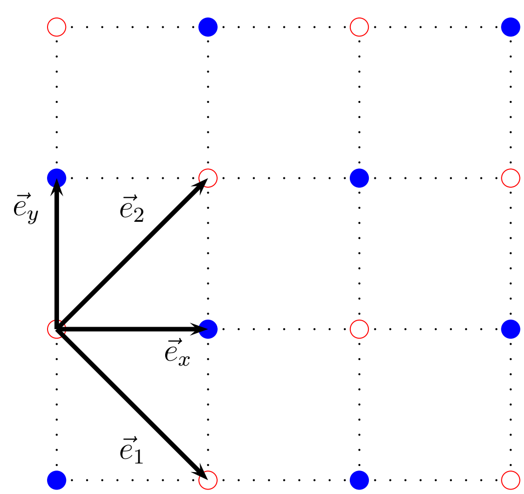


Figure B.1: Two dimensional bipartite lattice with the lattice basis $(\vec{e}_x, \vec{e}_y)$ and the spin sublattice basis $(\vec{e}_1, \vec{e}_2)$ in direct space.

If one sets the lattice parameter a to 1 the wave vector $\vec{k}$ is defined by

$$\vec{k} = k_1 \tilde{\vec{e}}_1 + k_2 \tilde{\vec{e}}_2 \tag{B.3}$$

$$k_1 = 2\pi \frac{l_1}{\mathcal{N}_{A(B),1}} \tag{B.4}$$

$$k_2 = 2\pi \frac{l_2}{\mathcal{N}_{A(B),2}} \tag{B.5}$$

where $\mathcal{N}_{A(B),1(2)}$ is the number of sublattice type-$A(B)$ sites in the direction 1(2) with $l_1 \in \left[-\frac{\mathcal{N}_{A(B),1}}{2}, \frac{\mathcal{N}_{A(B),1}}{2}\right] \in \mathbb{Z}$ and $l_2 \in \left[-\frac{\mathcal{N}_{A(B),2}}{2}, \frac{\mathcal{N}_{A(B),2}}{2}\right] \in \mathbb{Z}$ forming the Spin Brillouin Zone depicted in figure 4.2. The $\gamma_{\vec{k}}$ function defined in section 4.2.2 becomes

$$\begin{aligned}
\gamma_{\vec{k}} &= \frac{1}{z} \sum_{\vec{\eta}} e^{i\vec{k}.\vec{\eta}} \\
&= \frac{1}{2} \sum_{\vec{\eta}} \cos \vec{k}.\vec{\eta} \\
&= \cos\left(\frac{k_1 + k_2}{\sqrt{2}}\right) + \cos\left(\frac{k_1 - k_2}{\sqrt{2}}\right)
\end{aligned} \tag{B.6}$$

where $\vec{k}$ belongs to the Spin Brillouin Zone and $D = 2$. The total number of lattice sites is $\mathcal{N} = \mathcal{N}_{A,1}.\mathcal{N}_{A,2} + \mathcal{N}_{B,1}.\mathcal{N}_{B,2}$.

B.2 Three dimensional bipartite lattices

In three dimensions the direct spin sublattice is introduced for the bipartite lattice. For the Néel state a face-centered cubic lattice is used. The lattice basis $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$ reads

$$\vec{e}_1 = \frac{1}{\sqrt{2}} (\vec{e}_x + \vec{e}_y) \tag{B.7}$$

$$\vec{e}_2 = \frac{1}{\sqrt{2}} (\vec{e}_y + \vec{e}_z) \tag{B.8}$$

$$\vec{e}_3 = \frac{1}{\sqrt{2}} (\vec{e}_x + \vec{e}_z) \tag{B.9}$$

The reciprocal basis $\{\tilde{\vec{e}}_i\}$ of the lattice is defined by $\tilde{\vec{e}}_i.\vec{e}_j = \delta_{ij}$ and reads

$$\tilde{\vec{e}}_1 = \frac{\sqrt{2}}{2} (\vec{e}_x + \vec{e}_y - \vec{e}_z) \tag{B.10}$$

$$\tilde{\vec{e}}_2 = \frac{\sqrt{2}}{2} (-\vec{e}_x + \vec{e}_y + \vec{e}_z) \tag{B.11}$$

$$\tilde{\vec{e}}_3 = \frac{\sqrt{2}}{2} (\vec{e}_x - \vec{e}_y + \vec{e}_z) \tag{B.12}$$

These vectors are those of a body-centered cubic lattice. The wave vector $\vec{k}$ reads

$$\vec{k} = k_1\vec{\tilde{e}}_1 + k_2\vec{\tilde{e}}_2 + k_3\vec{\tilde{e}}_3 \tag{B.13}$$

$$k_i = 2\pi \frac{l_i}{\mathcal{N}_{A(B),i}} \tag{B.14}$$

$$l_i \in \left[-\frac{\mathcal{N}_{A(B),i}}{2}, \frac{\mathcal{N}_{A(B),i}}{2}\right] \in \mathbb{Z} \tag{B.15}$$

where $\mathcal{N}_{A(B),i}$ is the number of site in the direction $\vec{e}_i$ of the sublattice $A(B)$.

The $\gamma_{\vec{k}}$ function for $\vec{k}$ in the three dimensional Spin Brillouin Zone reads

$$\begin{aligned}\gamma_{\vec{k}} &= \frac{1}{z}\sum_{\vec{\eta}} e^{i\vec{k}.\vec{\eta}} \\ &= \frac{1}{3}\left[\cos\left(k_1 - k_2 + k_3\right) + \cos\left(k_1 + k_2 - k_3\right) + \cos\left(-k_1 + k_2 + k_3\right)\right] \end{aligned} \tag{B.16}$$

The total number of lattice is $\mathcal{N} = \prod_i \mathcal{N}_{A,i} + \prod_i \mathcal{N}_{B,i}$.

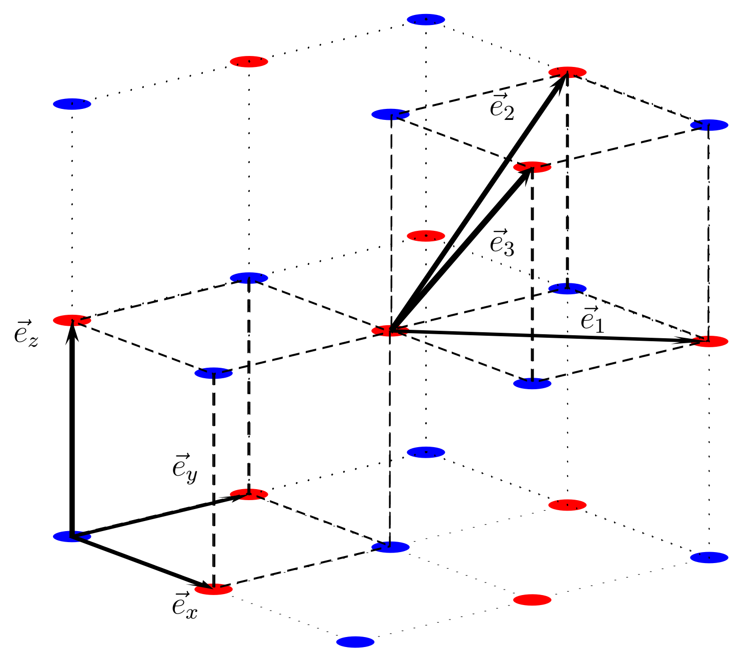


Figure B.2: Three dimensional bipartite lattice with direct space basis $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$

Figure B.2 shows a three dimensional bipartite lattice where blue points refer to one type of sublattice A and red points to the other type B. The crystal basis $(\vec{e}_x, \vec{e}_y, \vec{e}_z)$ as well as the direct basis $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$ are indicated.

Appendix C

Beyond the mean field : one-loop contributions

In section 4.3 we defined the mean-field contribution of the matrix M as

$$G_{0p,q} = \begin{bmatrix} -\frac{1}{\det G_p}\left[i\omega_{F,p} - \frac{1}{2}\bar{\varphi}_i^z(\omega_{F,p}-\omega_{F,q})\right]\delta_{p,q} & \frac{1}{\det G_p}\frac{1}{2}\bar{\varphi}_i^-(\omega_{F,p}-\omega_{F,q})\delta_{p,q} \\ \frac{1}{\det G_p}\frac{1}{2}\bar{\varphi}_i^+(\omega_{F,p}-\omega_{F,q})\delta_{p,q} & -\frac{1}{\det G_p}\left[i\omega_{F,p} + \frac{1}{2}\bar{\varphi}_i^z(\omega_{F,p}-\omega_{F,q})\right]\delta_{p,q} \end{bmatrix} \tag{C.1}$$

where $\det G_p = -\left[\widetilde{\omega}_{F,p}^2 + \left(\frac{\vec{\bar{\varphi}}_i(\frac{2\pi}{\beta}(p-q=0))}{2}\right)^2\right]$ and the contribution to the fluctuations $\delta\vec{\varphi}$ is given by

$$M_{1p,q} = \begin{bmatrix} \frac{1}{2}\delta\varphi_i^z(\omega_{F,p}-\omega_{F,q}) & \frac{1}{2}\delta\varphi_i^-(\omega_{F,p}-\omega_{F,q}) \\ \frac{1}{2}\delta\varphi_i^+(\omega_{F,p}-\omega_{F,q}) & -\frac{1}{2}\delta\varphi_i^z(\omega_{F,p}-\omega_{F,q}) \end{bmatrix} \tag{C.2}$$

It comes out that the term $\ln\det\beta M$ can be decomposed into a series expansion

$$\ln\det\beta M = -\sum_i \ln 2\cosh\frac{\beta}{2}\|\vec{\bar{\varphi}}_i(\omega_B=0)\| + Tr\{\sum_{n=1}^{\infty}\frac{1}{n}(G_0M_1)^n\} \tag{C.3}$$

where the fluctuation contributions appear in the second term of (C.3).

C.1 First order contributions to the fluctuations and mean-field equation

Here we aim to work out the $n=1$ contribution to the sum of $\ln\det\beta M$, $Tr\,[G_0M_1]$, and extract the mean-field equation with respect to the Hubbard-Stratonovich auxiliary mean-field $\bar{\varphi}$. The first order term in the fluctuations $\delta\varphi$ reads

$$[G_0 M_1]_{p,q} = \begin{bmatrix} A_i(p,q) & B_i(p,q) \\ C_i(p,q) & D_i(p,q) \end{bmatrix} \tag{C.4}$$

where i stands for the position on the spin lattice and p and q refer to the fermion Matsubara frequencies $\widetilde{\omega}_{F,p} \equiv \frac{2\pi}{\beta}(p+1/4)$ and similarly for $\widetilde{\omega}_{F,q}$. The matrix elements A, B, C and D are given by

$$\begin{aligned}
A_i(p,q) &= \Bigg[-\frac{1}{2\det G_p}\left[\widetilde{\omega}_{F,p} - \frac{\bar{\varphi}_i^z}{2}(\frac{2\pi}{\beta}(p-q=0))\right]\delta\varphi_i^z(\frac{2\pi}{\beta}(p-q)) \\
&+ \frac{1}{2\det G_p}\frac{\bar{\varphi}_i^-}{2}(\frac{2\pi}{\beta}(p-q=0))\delta\varphi_i^+(\frac{2\pi}{\beta}(p-q))\Bigg] \qquad (C.5) \\
B_i(p,q) &= \Bigg[-\frac{1}{2\det G_p}\left[\widetilde{\omega}_{F,p} - \frac{\bar{\varphi}_i^z}{2}(\frac{2\pi}{\beta}(p-q=0))\right]\delta\varphi_i^-(\frac{2\pi}{\beta}(p-q)) \\
&- \frac{1}{2\det G_p}\frac{\bar{\varphi}_i^-}{2}(\frac{2\pi}{\beta}(p-q=0))\delta\varphi_i^z(\frac{2\pi}{\beta}(p-q))\Bigg] \qquad (C.6) \\
C_i(p,q) &= \Bigg[\frac{1}{2\det G_p}\frac{\bar{\varphi}_i^+}{2}(\frac{2\pi}{\beta}(p-q=0))\delta\varphi_i^z(\frac{2\pi}{\beta}(p-q)) \\
&- \frac{1}{2\det G_p}\left[\widetilde{\omega}_{F,p} + \frac{\bar{\varphi}_i^z}{2}(\frac{2\pi}{\beta}(p-q=0))\right]\delta\varphi_i^+(\frac{2\pi}{\beta}(p-q))\Bigg] \qquad (C.7) \\
D_i(p,q) &= \Bigg[\frac{1}{2\det G_p}\frac{\bar{\varphi}_i^+}{2}(\frac{2\pi}{\beta}(p-q=0))\delta\varphi_i^-(\frac{2\pi}{\beta}(p-q)) \\
&- \frac{1}{2\det G_p}\left[\widetilde{\omega}_{F,p} + \frac{\bar{\varphi}_i^z}{2}(\frac{2\pi}{\beta}(p-q=0))\right]\delta\varphi_i^z(\frac{2\pi}{\beta}(p-q))\Bigg] \qquad (C.8)
\end{aligned}$$

The first term in the sum of $\ln\det\beta M$ reads

$$\begin{aligned}
Tr\,[G_0 M_1] &= \sum_i \sum_p [A_i(p,p) + D_i(p,p)] \\
&= \sum_i \sum_p \frac{1}{2\det G_p}\left[\bar{\varphi}_i^z(0)\delta\varphi_i^z(0) + \frac{1}{2}\left(\bar{\varphi}_i^+(0)\delta\varphi_i^-(0) + \bar{\varphi}_i^-(0)\delta\varphi_i^+(0)\right)\right] \\
&= \sum_i \left(\sum_p \frac{1}{2\det G_p}\right)\vec{\bar{\varphi}}_i(0)\delta\vec{\varphi}_i(0) \qquad (C.9)
\end{aligned}$$

The value of $\left(\sum_p \frac{1}{2\det G_p}\right)$ can be found with the help of the sum relation in [30] and leads to

$$Tr\left[G_0M_1\right] = -\frac{\beta}{2}\sum_i \tanh\left(\frac{\beta}{2}\|\vec{\bar{\varphi}}_i(0)\|\right)\frac{\vec{\bar{\varphi}}_i}{\bar{\varphi}_i(0)}.\delta\vec{\varphi}_i(0) \tag{C.10}$$

The first term in order of the fluctuations $\delta\vec{\varphi}$ of the auxiliary field action $S_0\left[\varphi\right]$ in equation (4.43) reads

$$\begin{aligned}
\left.\frac{\delta S_0\left[\varphi\right]}{\delta\vec{\varphi}}\right|_{\delta\vec{\varphi}=0} &= \frac{\delta}{\delta\vec{\varphi}}\left[\frac{\beta}{2}\sum_{\omega_B}\sum_{i,j}J_{ij}^{-1}\left[\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right)\delta(\omega_B=0) + \delta\vec{\varphi}_i(-\omega_B)\right].\right. \\
&\quad \left.\left.\left[\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right)\delta(\omega_B=0) + \delta\vec{\varphi}_j(\omega_B)\right]\right]\right|_{\delta\vec{\varphi}=0} \\
&= \frac{\beta}{2}\sum_{i,j}J_{ij}^{-1}\left[\left(\vec{\bar{\varphi}}_i - \vec{B}_i\right)\delta\vec{\varphi}_i(0) + \left(\vec{\bar{\varphi}}_j - \vec{B}_j\right)\delta\vec{\varphi}_j(0)\right] \qquad \text{(C.11)}
\end{aligned}$$

Adding the first order term in the fluctuations $\delta\varphi$ of $S_0\left[\varphi\right]$ in (C.10) leads to

$$\begin{aligned}
\left.\frac{\delta S_{eff}}{\delta\vec{\varphi}}\right|_{[\vec{\bar{\varphi}}]}\delta\vec{\varphi} &= \frac{\delta S_0\left[\varphi\right]}{\delta\vec{\varphi}}\delta\vec{\varphi} \\
&= \frac{\beta}{2}\sum_i\left[2\sum_j J_{ij}^{-1}\left(\vec{\bar{\varphi}}_j - \vec{B}_j\right) - \frac{\vec{\bar{\varphi}}_i}{\|\,\vec{\bar{\varphi}}_i\|}\tanh\left(\frac{\beta}{2}\|\vec{\bar{\varphi}}_i\|\right)\right].\delta\vec{\varphi}_i(\omega_B=0) = 0
\end{aligned} \tag{C.12}$$

From (C.12) one obtains directly the mean-field equation of the Hubbard-Stratonovich equation (4.46).

C.2 Second order fluctuation contributions

The term $n = 2$ in equation (4.43) is given by

$$
\begin{aligned}
Tr\left[G_0 M_1 G_0 M_1\right] &= \sum_i \sum_{p,q} \Big[A_i(p,q)A_i(q,p) + B_i(p,q)C_i(q,p) \\
&+ C_i(p,q)B_i(q,p) + D_i(p,q)D_i(q,p) \Big] \\
&= \sum_i \sum_{\omega_B} \frac{1}{4}\left[\left(\bar\varphi^+/2\right)^2 \mathcal{K}_{i,\omega_B}\right] \delta\varphi_i^-(-\omega_B)\delta\varphi_i^-(\omega_B) \\
&+ \frac{1}{4}\left[\left(\bar\varphi^-/2\right)^2 \mathcal{K}_{i,\omega_B}\right] \delta\varphi_i^+(-\omega_B)\delta\varphi_i^+(\omega_B) \\
&+ \frac{1}{2}\left[\frac{1}{4}\left((\bar\varphi_i^z)^2 - \bar\varphi_i^+\bar\varphi_i^-\right)\mathcal{K}_{i,\omega_B} - \mathcal{I}_{i,\omega_B}\right] \delta\varphi_i^z(-\omega_B).\delta\varphi_i^z(\omega_B) \\
&- \frac{1}{2}\left[\frac{\bar\varphi_i^z}{2}\left(\frac{\bar\varphi_i^z}{2} + i\omega_B\right)\mathcal{K}_{i,\omega_B} + \mathcal{I}_{i,\omega_B}\right] \delta\varphi_i^-(-\omega_B)\delta\varphi_i^+(\omega_B) \\
&+ \frac{1}{4}\left[\bar\varphi_i^-\left(\bar\varphi_i^z + i\omega_B\right)\mathcal{K}_{i,\omega_B}\right] \delta\varphi_i^z(-\omega_B)\delta\varphi_i^+(\omega_B) \\
&+ \frac{1}{4}\left[\bar\varphi_i^+\left(\bar\varphi_i^z - i\omega_B\right)\mathcal{K}_{i,\omega_B}\right] \delta\varphi_i^z(-\omega_B)\delta\varphi_i^-(\omega_B) \qquad \text{(C.13)}
\end{aligned}
$$

where $\omega_B = \widetilde{\omega}_{F,p} - \widetilde{\omega}_{F,q} = \frac{2\pi(p-q)}{\beta}$ and we define $\mathcal{K}_{i,\omega_B}$ and $\mathcal{I}_{i,\omega_B}$ by

$$
\begin{aligned}
\mathcal{K}_{i,\omega_B} &= \sum_{\omega_{F,p}} \frac{1}{\det G_{\omega_{F,p}}.\det G_{\omega_{F,p}+\omega_B}} \\
&= \begin{cases} -\frac{1}{\bar\varphi}\frac{d}{d\bar\varphi_i}\left[\frac{\beta}{\bar\varphi_i}\tanh\frac{\beta}{2}\bar\varphi_i\right] & \text{, when } \omega_B = 0, \\ \frac{2\beta}{\bar\varphi_i(\bar\varphi_i)^2+\omega_B^2}\tanh\frac{\beta}{2}\bar\varphi_i & \text{, when } \omega_B \neq 0. \end{cases} \qquad \text{(C.14)}
\end{aligned}
$$

and

$$
\begin{aligned}
\mathcal{I}_{i,\omega_B} &= \sum_{\omega_{F,p}} \frac{\omega_{F,p}(\omega_{F,p}+\omega_B)}{\det G_{\omega_{F,p}}.\det G_{\omega_{F,p}+\omega_B}} \\
&= \begin{cases} \frac{\beta}{2\bar\varphi_i}\tanh\frac{\beta}{2}\bar\varphi_i + \frac{\beta^2}{4}\tanh'\frac{\beta}{2}\bar\varphi_i & \text{, when } \omega_B = 0, \\ \frac{\beta}{2\bar\varphi_i}\tanh\frac{\beta}{2}\bar\varphi_i - \left(\frac{\omega_B}{2}\right)^2\mathcal{K}_{i,\omega_B} & \text{, when } \omega_B \neq 0. \end{cases} \qquad \text{(C.15)}
\end{aligned}
$$

Gathering all terms of second order with respect to the fluctuations $\delta\varphi$ from (4.43) one gets (4.52) if the mean-field $\bar\varphi$ is of a Néel or ferromagnetic type ($\bar\varphi^+ = \bar\varphi^- = 0$ and $\bar\varphi^z \neq 0$).

C.3 Derivation of the free energy with fluctuation contributions

From relations (4.52) one can define

$$① = \left(\frac{\beta}{4}\tanh'\left(\frac{\beta}{2}\bar{\varphi}_i^z\right)\right) \tag{C.16}$$

and

$$② = \left(\frac{1}{2}\frac{\tanh\left(\frac{\beta}{2}\bar{\varphi}_i^z\right)}{\bar{\varphi}_i^z - i\omega_B}\right) \tag{C.17}$$

Using relations (4.55) and (4.56) with $\bar{m}_i = (-1)^i\bar{m} + \Delta m B_i$, ① and ② read

$$\begin{aligned}
① &= \left(\frac{\beta}{4}\tanh'\left(\frac{\beta}{2}\bar{\varphi}_\alpha^z\right)\right) \\
&= \frac{\beta}{4}\left(1-4\bar{m}_i^2\right) \\
&= [1a] + [1b]\,(-1)^{\vec{r}_i.\vec{\pi}} \\
&= \begin{cases} \frac{\beta}{4}\left(1-4\left(\bar{m}+\Delta\tilde{m}_0.B\right)^2\right) & \text{, when } B_i = (-1)^{\vec{r}_i.\vec{\pi}} \\ \frac{\beta}{4}\left(1-4\left(\bar{m}^2+(\Delta\tilde{m}_0.B)^2\right)\right) - 2\beta\Delta m_{\chi 0}.B\bar{m}(-1)^{\vec{r}_i.\vec{\pi}} & \text{, when } B_i = B. \end{cases}
\end{aligned} \tag{C.18}$$

and

$$\begin{aligned}
② &= \left(\frac{1}{2}\frac{\tanh\left(\frac{\beta}{2}\bar{\varphi}_\alpha^z\right)}{\bar{\varphi}_\alpha^z - i\omega_B}\right) \\
&= [2a]_{\omega_B} + (-1)^{\vec{r}_i.\vec{\pi}}\,[2b]_{\omega_B}
\end{aligned}$$

where

$$[2a]_{\omega_B} = \frac{(\bar{m}+\Delta\tilde{m}_0.B).(B+2D|J|(\bar{m}+\Delta\tilde{m}_0.B))}{[(B+2D|J|(\bar{m}+\Delta\tilde{m}_0.B))^2+\omega_B{}^2]} \tag{C.19}$$

$$[2b]_{\omega_B} = \frac{i\omega(\bar{m}+\Delta\tilde{m}_0.B)}{[(B+2D|J|(\bar{m}+\Delta\tilde{m}_0.B))^2+\omega_B{}^2]} \tag{C.20}$$

if $B_i = (-1)^{\vec{r}_i.\vec{\pi}}$ and

$$[2a]_{\omega_B} = \frac{\Delta m_{\chi 0}.B\left(B-2|J|B.\Delta m_{\chi 0}-i\omega_B\right)-2|J|\bar{m}^2}{\left(B-2|J|\Delta m_{\chi 0}.B\right)^2-\left(2|J|\bar{m}\right)^2} \tag{C.21}$$

$$[2b]_{\omega_B} = \frac{\bar{m}\left(B-2|J|B.\Delta m_{\chi 0}-i\omega_B\right)-2|J|\bar{m}.\Delta m_{\chi 0}.B}{\left(B-2|J|\Delta m_{\chi 0}.B\right)^2-\left(2|J|\bar{m}\right)^2} \tag{C.22}$$

if $B_i = B$. After these developments in equations (4.52), the use of a Fourier transformation and integration over the Hubbard-Stratonovich auxiliary field $\delta\vec{\varphi}$ equations (4.49) and (4.50) come out as

$$\mathcal{Z}_{zz} = \prod_{\vec{k}\in SBZ} \det \begin{bmatrix} \left(1 - [1a]\, J(\vec{k})\right) & -[1b]\, J(\vec{k}+\vec{\pi}) \\ -[1b]\, J(\vec{k}) & \left(1 - [1a]\, J(\vec{k}+\vec{\pi})\right) \end{bmatrix}^{-1/2} \tag{C.23}$$

$$\mathcal{Z}_{+-} = \prod_{\omega_B}\prod_{\vec{k}\in SBZ} \det \begin{bmatrix} \left(1 - [2a]_{\omega_B}\, J(\vec{k})\right) & -[2b]_{\omega_B}\, J(\vec{k}+\vec{\pi}) \\ -[2b]_{\omega_B}\, J(\vec{k}) & \left(1 - [2a]_{\omega_B}\, J(\vec{k}+\vec{\pi})\right) \end{bmatrix}^{-1} \tag{C.24}$$

Here $J(\vec{k}) \equiv -Z|J|\gamma_{\vec{k}}$ and $\vec{\pi}$ is the Brioullin vector relative to the spin lattice as defined in section 4.2. Then free energy components $\mathcal{F}_{MF}$, $\mathcal{F}_{zz}$ and $\mathcal{F}_{+-}$ are given by

$$\mathcal{F}_{MF} = \mathcal{N} D|J|\left(\bar{m} + \Delta\tilde{m}_0.B\right)^2 - \frac{\mathcal{N}}{\beta}\ln\cosh\left(\frac{\beta}{2}\left[B + 2D|J|(\bar{m} + \Delta\tilde{m}_0.B)\right]\right) \tag{C.25}$$

$$\mathcal{F}_{zz} = \frac{1}{2\beta}\sum_{\vec{k}\in SBZ} \ln\left[1 - \left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2 \left[1 - 4(\bar{m} + \Delta\tilde{m}_0.B)^2\right]^2\right] \tag{C.26}$$

$$\mathcal{F}_{+-} = \frac{2}{\beta}\sum_{\vec{k}\in SBZ} \ln\left(\frac{\sinh\left(\frac{\beta}{2}\left(\left[B + 2D|J|(\bar{m} + \Delta\tilde{m}_0.B)\right]^2 - \left[2D|J|\gamma_{\vec{k}}(\bar{m} + \Delta\tilde{m}_0.B)\right]^2\right)^{1/2}\right)}{\sinh\left(\frac{\beta}{2}\left[B + 2D|J|(\bar{m} + \Delta\tilde{m}_0.B)\right]\right)} \right) \tag{C.27}$$

if the magnetic field B_i is equal to $(-1)^{\vec{r}_i.\vec{\pi}}B$ and

$$\begin{aligned}\mathcal{F}_{MF} =& \mathcal{N} D|J|\left(\bar{m}^2 - (\Delta m_{\chi 0}.B)^2\right) \\ & -\frac{\mathcal{N}}{2\beta}\ln\left(\cosh\left[\frac{\beta}{2}\left((1 - 2D|J|\Delta m_{\chi 0}).B + 2D|J|\bar{m}\right)\right]\right. \\ & \left. .\cosh\left[\frac{\beta}{2}\left((1 - 2D|J|\Delta m_{\chi 0}).B - 2D|J|\bar{m}\right)\right]\right)\end{aligned} \tag{C.28}$$

$$\mathcal{F}_{zz} = \frac{1}{2\beta}\sum_{\vec{k}\in SBZ} \ln\left[1-\left(\frac{\beta D|J|\gamma_{\vec{k}}}{2}\right)^2\left[1-4(\bar{m}-\Delta m_{\chi 0}.B)^2\right]\left[1-4(\bar{m}+\Delta m_{\chi 0}.B)^2\right]\right] \tag{C.29}$$

$$\mathcal{F}_{+-} = \frac{1}{\beta}\sum_{\vec{k}\in SBZ} \ln\left[\frac{\sinh^2\left(\beta D|J|\bar{m}\sqrt{1-\gamma_{\vec{k}}^2\left[1-(\frac{\Delta m_{\chi 0}.B}{\bar{m}})^2\right]}\right) - \sinh^2\frac{\beta}{2}((1-2D|J|\Delta m_{\chi 0}).B)}{\sinh^2\beta D|J|\bar{m} - \sinh^2\frac{\beta}{2}((1-2D|J|\Delta m_{\chi 0}).B)}\right] \tag{C.30}$$

if the magnetic field B_i is unform and equal to B. Here $\mathcal{N}$ is the number of lattice sites (sublattices A and B). The magnetization of the spin system is obtained by means of (C.25), (C.26) and (C.27). The magnetic spin susceptibility can be worked out with (C.28), (C.29) and (C.30).

C.4 The free energy of the XXZ-model with a staggered magnetic field

The free energy of the XXZ-model in a staggered magnetic field $B_i = (-1)^i B$ is given by the three contributions $\mathcal{F}_{MF}$, $\mathcal{F}_{zz}$ and $\mathcal{F}_{+-}$ where

$$\begin{aligned}\mathcal{F}_{MF} &= \mathcal{N}D|J(1+\delta)|\left(\bar{m}+\Delta\tilde{m}_{XXZ}.B\right)^2 \\ &- \frac{\mathcal{N}}{\beta}\ln\cosh\left(\frac{\beta}{2}\left[B+2D|J(1+\delta)|(\bar{m}+\Delta\tilde{m}_{XXZ}.B)\right]\right)\end{aligned} \tag{C.31}$$

$$\delta\mathcal{F}_{zz} = \frac{1}{2\beta}\sum_{\vec{k}\in SBZ} \ln\left[1-\left(\frac{\beta D|J(1+\delta)|\gamma_{\vec{k}}}{2}\right)^2\left[1-4(\bar{m}+\Delta\tilde{m}_{XXZ}.B)^2\right]^2\right] \tag{C.32}$$

$$\delta\mathcal{F}_{+-} = \frac{2}{\beta}\sum_{\vec{k}\in SBZ}\ln\Bigg(\frac{\sinh\left(\frac{\beta}{2}\left(\left[B+2D|J(1+\delta)|(\bar{m}+\Delta\tilde{m}_{XXZ}.B)\right]^2-\left[2D|J|\gamma_{\vec{k}}(\bar{m}+\Delta\tilde{m}_{XXZ}.B)\right]^2\right)^{1/2}\right)}{\sinh\left(\frac{\beta}{2}\left[B+2D|J(1+\delta)|(\bar{m}+\Delta\tilde{m}_{XXZ}.B)\right]\right)}\Bigg) \tag{C.33}$$

Appendix D

Diagonalization of Mean-Field Hamiltonians

D.1 Bogoliubov transformation on the Néel mean-field Hamiltonian

The Néel mean-field Hamiltonian (5.11)

$$\begin{aligned}\mathcal{H}_{MF} &= -\frac{1}{2}\sum_{i,j} J^{-1}_{ij}\left(\vec{\bar{\varphi}}_i - B_i\vec{e}_z\right).\left(\vec{\bar{\varphi}}_j - B_j\vec{e}_z\right) \\ &+ \sum_i \left(\begin{array}{cc} f^\dagger_{i,\uparrow} & f^\dagger_{i,\downarrow} \end{array}\right) \left[\begin{array}{cc} \left(-\mu + \frac{\bar{\varphi}^z_i}{2}\right) & \frac{\bar{\varphi}^-_i}{2} \\ \frac{\bar{\varphi}^+_i}{2} & -\left(\mu + \frac{\bar{\varphi}^z_i}{2}\right) \end{array}\right] \left(\begin{array}{c} f_{i,\uparrow} \\ f_{i,\downarrow} \end{array}\right)\end{aligned} \tag{D.1}$$

can be diagonalized by means of a Bogoliubov tranformation [15]. Introduce the linar combination of new creation and annihilation fermion operators $\beta^\dagger_{i,(\pm)}$ and $\beta_{i,(\pm)}$

$$\left(\begin{array}{c} f_{i,\uparrow} \\ f_{i,\downarrow} \end{array}\right) = U \left(\begin{array}{c} \beta_{i,(+)} \\ \beta_{i,(-)} \end{array}\right) \tag{D.2}$$

where the unitary matrix U is define by

$$U = \left[\begin{array}{cc} u_i & v^*_i \\ -v_i & u^*_i \end{array}\right] \tag{D.3}$$

Coefficients $\{u_i\}$ and $\{v_i\}$ have to verify $\det U = 1$ and $U^{-1} = U^\dagger$ in such a way that in the transformation (D.2) the creation and annihilation operator $\{\beta^\dagger_{i,(\pm)}\}$ and $\{\beta_{i,(\pm)}\}$ anticommute. To diagonalize the Hamiltonian (5.10) one should find the coefficients $\{u_i\}$ and $\{v_i\}$ for which

$$
\begin{aligned}
U^{-1}\mathcal{H}_{MF}U &= U^{\dagger}\mathcal{H}_{MF}U \\
&= -\frac{1}{2}\sum_{i,j} J_{ij}^{-1}\left(\vec{\bar{\varphi}}_i - B_i\vec{e}_z\right).\left(\vec{\bar{\varphi}}_j - B_j\vec{e}_z\right) \\
&+ \sum_i \begin{pmatrix} \beta^{\dagger}_{i,(+)} & \beta^{\dagger}_{i,(-)} \end{pmatrix} \begin{bmatrix} \omega^{(PFP)}_{i,(+)} & 0 \\ 0 & \omega^{(PFP)}_{i,(-)} \end{bmatrix} \begin{pmatrix} \beta_{i,(+)} \\ \beta_{i,(-)} \end{pmatrix}
\end{aligned}
\tag{D.4}
$$

By means of the transformation

$$
\begin{cases} u_i = e^{i\alpha_i}\cos\theta_i \\ v_i = \sin\theta_i \end{cases}
\tag{D.5}
$$

where α_i and θ_i are angles, $U^{\dagger}\mathcal{H}_{MF}U$ is diagonal for

$$
\tan\alpha_i = -\frac{\bar{\varphi}^y_i}{\bar{\varphi}^x_i} \tag{D.6}
$$

$$
\tan 2\theta_i = -\frac{\sqrt{(\bar{\varphi}^x_i)^2 + (\bar{\varphi}^y_i)^2}}{\bar{\varphi}^z_i} \tag{D.7}
$$

And then

$$
U^{\dagger}\mathcal{H}_{MF}U = \begin{bmatrix} \omega^{(PFP)}_{i,(+)} & 0 \\ 0 & \omega^{(PFP)}_{i,(-)} \end{bmatrix} \tag{D.8}
$$

with $\omega^{(PFP)}_{i,(\pm)} = \mu \pm \frac{\|\vec{\bar{\varphi}}\|}{2}$, ($PFP$ refers to the Popov and Fedotov procedure).

D.2 Bogoliubov transformation on Diffuson mean-field ansatz

The mean-field Hamiltonian (5.39) with the imaginary chemical potential fixing exactly the number of spin per lattice site given by

$$
\begin{aligned}
\mathcal{H}^{(PFP)}_{MF} &= \mathcal{N}z\frac{\Delta^2}{|J|} + \sum_{\vec{k}\in SBZ}\sum_{\sigma}\left(f^{\dagger}_{\vec{k},\sigma}\, f^{\dagger}_{\vec{k}+\vec{\pi},\sigma}\right) \\
& \begin{bmatrix} -\mu + \Delta\cos\frac{\pi}{4}z\gamma_{k_x,k_y} & -i\Delta\sin\frac{\pi}{4}z\gamma_{k_x,k_y+\pi} \\ +i\Delta\sin\frac{\pi}{4}z\gamma_{k_x,k_y+\pi} & -\mu - \Delta\cos\frac{\pi}{4}z\gamma_{k_x,k_y} \end{bmatrix} \begin{pmatrix} f_{\vec{k},\sigma} \\ f_{\vec{k}+\vec{\pi},\sigma} \end{pmatrix}
\end{aligned}
\tag{D.9}
$$

can be diagonalized by the transformation (D.3)

$$\begin{pmatrix} f_{\vec{k},\sigma} \\ f_{\vec{k}+\vec{\pi},\sigma} \end{pmatrix} = \begin{bmatrix} u_{\vec{k}} & v^*_{\vec{k}} \\ -v_{\vec{k}} & u^*_{\vec{k}} \end{bmatrix} \begin{pmatrix} \beta_{(+),\vec{k},\sigma} \\ \beta_{(-),\vec{k},\sigma} \end{pmatrix} \tag{D.10}$$

The transformation matrix

$$U = \begin{bmatrix} u_{\vec{k}} & v^*_{\vec{k}} \\ -v_{\vec{k}} & u^*_{\vec{k}} \end{bmatrix} \tag{D.11}$$

is unitary and

$$|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1 \tag{D.12}$$

so that $\beta^\dagger$ and β are fermion creation and annihilation operator. Following the section D.1 we define

$$\begin{aligned} u_{\vec{k}} &= e^{i\varphi_{\vec{k}}} \cos\theta_{\vec{k}} && \text{(D.13)} \\ v_{\vec{k}} &= \sin\theta_{\vec{k}} && \text{(D.14)} \end{aligned}$$

The mean-field Hamiltonian is diagonal if

$$\begin{aligned} \varphi_{\vec{k}} &= \frac{\pi}{2} && \text{(D.15)} \\ \tan 2\theta_{\vec{k}} &= \frac{\gamma_{k_x,k_x+\pi}}{\gamma_{k_x,k_y}} && \text{(D.16)} \end{aligned}$$

where $\gamma_{\vec{k}} = \frac{1}{2}(\cos k_x + \cos k_y)$ and reads

$$\mathcal{H}^{(PFP)}_{MF} = \mathcal{N}\frac{z\Delta^2}{|J|} + \sum_{\vec{k}\in SBZ}\sum_{\sigma}\left[\omega^{(PFP)}_{(+),\vec{k},\sigma}\beta^\dagger_{(+),\vec{k},\sigma}\beta_{(+),\vec{k},\sigma} + \omega^{(PFP)}_{(-),\vec{k},\sigma}\beta^\dagger_{(-),\vec{k},\sigma}\beta_{(-),\vec{k},\sigma}\right] \tag{D.17}$$

with

$$\begin{aligned} \omega^{(PFP)}_{(+),\vec{k},\sigma} &= -\mu + 2\Delta\sqrt{\cos^2 k_x + \cos^2 k_y} && \text{(D.18)} \\ \omega^{(PFP)}_{(-),\vec{k},\sigma} &= -\mu - 2\Delta\sqrt{\cos^2 k_x + \cos^2 k_y} && \text{(D.19)} \end{aligned}$$

D.3 Bogoliubov transformation on Cooperon mean-field ansatz

The mean-field Hamiltonian (5.60) describing the cooperon mean-field ansatz with exact occupation parameter μ is given by

$$\mathcal{H}_{MF}^{(PFP)} = \mathcal{N}\frac{z\Gamma^2}{|J|} - \sum_{\vec{k}\in BZ,\sigma}\left[\mu f^\dagger_{\vec{k},\sigma} f_{\vec{k},\sigma} + \sigma\frac{z\Gamma\gamma_{\vec{k}}}{2}\left(f_{\vec{k},\sigma} f_{-\vec{k},-\sigma} - f^\dagger_{\vec{k},\sigma} f^\dagger_{-\vec{k},-\sigma}\right)\right] \tag{D.20}$$

and rewritten as

$$\mathcal{H}_{MF}^{(PFP)} = \mathcal{N}\frac{z\Gamma^2}{|J|} - \mathcal{N}\mu + \sum_{\vec{k}\in BZ}\left(\begin{array}{cc} f^\dagger_{\vec{k},\sigma} & f_{-\vec{k},-\sigma}\end{array}\right)\left[\begin{array}{cc} H_{11,\vec{k},\sigma} & H_{12,\vec{k},\sigma} \\ H_{21,\vec{k},\sigma} & H_{22,\vec{k},\sigma}\end{array}\right]\left(\begin{array}{c} f_{\vec{k},\sigma} \\ f^\dagger_{-\vec{k},-\sigma}\end{array}\right) \tag{D.21}$$

where

$$\begin{aligned} H_{11,\vec{k},\sigma} &= \frac{\mu}{2} && \text{(D.22)} \\ H_{12,\vec{k},\sigma} &= -\sigma\frac{z\Gamma\gamma_{\vec{k}}}{2} && \text{(D.23)} \\ H_{21,\vec{k},\sigma} &= -\sigma\frac{z\Gamma\gamma_{\vec{k}}}{2} && \text{(D.24)} \\ H_{22,\vec{k},\sigma} &= -\frac{\mu}{2} && \text{(D.25)} \end{aligned}$$

Following the same step as in section D.2 one define the Bogoliubov transformation

$$\left(\begin{array}{c} f_{\vec{k},\sigma} \\ f^\dagger_{-\vec{k},-\sigma}\end{array}\right) = U\left(\begin{array}{c} \beta_{\vec{k},\sigma} \\ \beta^\dagger_{-\vec{k},-\sigma}\end{array}\right) \tag{D.26}$$

where U is the unitary matrix

$$U = \left[\begin{array}{cc} u_{\vec{k}} & v^*_{\vec{k}} \\ -v_{\vec{k}} & u^*_{\vec{k}}\end{array}\right] \tag{D.27}$$

The coefficients verify $|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1$ and

$$\begin{aligned} u_{\vec{k}} &= e^{i\varphi_{\vec{k}}}\cos\theta_{\vec{k}} \\ v_{\vec{k}} &= \sin\theta_{\vec{k}} \end{aligned} \tag{D.28}$$

In order to diagonalize the mean-field Hamiltonian one looks for angles $\theta_{\vec{k}}$ and $\varphi_{\vec{k}}$ such that

$$U^{-1}\mathcal{H}_{MF}^{(PFP)}U = \begin{pmatrix} \beta^\dagger_{\vec{k},\sigma} & \beta_{-\vec{k},-\sigma} \end{pmatrix} \begin{bmatrix} \omega^{(PFP)}_{(+),\vec{k},\sigma} & 0 \\ 0 & \omega^{(PFP)}_{(-),\vec{k},\sigma} \end{bmatrix} \begin{pmatrix} \beta_{\vec{k},\sigma} \\ \beta^\dagger_{-\vec{k},-\sigma} \end{pmatrix} \tag{D.29}$$

Developing $U^{-1}\mathcal{H}_{MF}^{(PFP)}U$ in detail one gets the system of equations

$$\begin{cases} ① : & H_{11}u^*_{\vec{k}}u_{\vec{k}} - H_{12}u^*_{\vec{k}}v_{\vec{k}} - H_{21}u_{\vec{k}}v^*_{\vec{k}} + H_{22}v^*_{\vec{k}}v_{\vec{k}} = \omega^{(PFP)}_{(+),\vec{k},\sigma} \\ ② : & H_{11}v^*_{\vec{k}}v_{\vec{k}} + H_{12}u^*_{\vec{k}}v_{\vec{k}} + H_{21}u_{\vec{k}}v^*_{\vec{k}} + H_{22}v^*_{\vec{k}}v_{\vec{k}} = \omega^{(PFP)}_{(-),\vec{k},\sigma} \\ ③ : & H_{11}u^*_{\vec{k}}v^*_{\vec{k}} + H_{12}(u^*_{\vec{k}})^2 - H_{21}(v^*_{\vec{k}})^2 - H_{22}v^*_{\vec{k}}u^*_{\vec{k}} = 0 \\ ④ : & H_{11}u_{\vec{k}}v_{\vec{k}} - H_{12}(v_{\vec{k}})^2 + H_{21}(u_{\vec{k}})^2 - H_{22}v_{\vec{k}}u_{\vec{k}} = 0 \end{cases} \tag{D.30}$$

Introducing (D.28) in ③ and ④ leads to

$$③ \quad : \qquad H_{11}e^{-i\varphi_{\vec{k}}}.2\cos\theta_{\vec{k}}\sin\theta_{\vec{k}} + H_{12}\left(e^{-2i\varphi_{\vec{k}}}\cos^2\theta_{\vec{k}} - \sin^2\theta_{\vec{k}}\right) = 0 \tag{D.31}$$

$$④ \quad : \qquad H_{11}e^{i\varphi_{\vec{k}}}.2\cos\theta_{\vec{k}}\sin\theta_{\vec{k}} + H_{12}\left(e^{2i\varphi_{\vec{k}}}\cos^2\theta_{\vec{k}} - \sin^2\theta_{\vec{k}}\right) = 0 \tag{D.32}$$

Separating real and imaginary part one gets

$$\begin{array}{lccc} & \mathcal{R}\text{e part} & & \mathcal{I}\text{m part} \\ ③ : & H_{12}\cos 2\theta_{\vec{k}}\cos\varphi_{\vec{k}} = 0 & \text{and} & \frac{\mathcal{I}m(\mu)}{2}\sin 2\theta_{\vec{k}} - H_{12}\sin\varphi_{\vec{k}} = 0 \\ ④ : & H_{12}\cos 2\theta_{\vec{k}}\cos\varphi_{\vec{k}} = 0 & \text{and} & \frac{\mathcal{I}m(\mu)}{2}\sin 2\theta_{\vec{k}} + H_{12}\sin\varphi_{\vec{k}} = 0 \end{array} \tag{D.33}$$

Equation ③ and ④ cannot be verified simultaneously. As a consequence there is no unitary matrix U and hence no Bogoliubov transformation which can diagonalize the mean-field Hamiltonian (5.60). The mean-field Hamiltonian of the cooperon does not conserve the number of particles and hence gets in conflict with the Popov and Fedotov procedure which fixes the number of particles strictly.

Appendix E

Derivation of the QED_3 action and the polarization function at finite temperature

E.1 Derivation of the Euclidean QED action in (2+1) dimensions

At low energy near the two independent points $\vec{k} = \left(\pm\frac{\pi}{2}, \frac{\pi}{2}\right) + \vec{k}$ of the Spin Brillouin Zone (see figure 4.2) the Hamiltonian (6.5) can be rewritten in the form

$$
\begin{aligned}
H &= \sum_{\vec{k}\in SBZ} \sum_{\sigma} \left(f^{\dagger}_{1,\vec{k},\sigma}\, f^{\dagger}_{1,\vec{k}+\vec{\pi},\sigma}\, f^{\dagger}_{2,\vec{k},\sigma}\, f^{\dagger}_{2,\vec{k}+\vec{\pi},\sigma} \right) \\
& \Bigg\{ \quad -\mu \mathbb{I} + \sqrt{2}\Delta \left[-k_x \begin{pmatrix} \tau_3 & 0 \\ 0 & \tau_3 \end{pmatrix} - k_y \mathbb{I} \right] \\
&+ \quad \sqrt{2}\Delta \left[-k_x \begin{pmatrix} \tau_2 & 0 \\ 0 & -\tau_2 \end{pmatrix} + k_y . i \mathbb{I} \right] \Bigg\} \begin{pmatrix} f_{1,\vec{k},\sigma} \\ f_{1,\vec{k}+\vec{\pi},\sigma} \\ f_{2,\vec{k},\sigma} \\ f_{2,\vec{k}+\vec{\pi},\sigma} \end{pmatrix}
\end{aligned}
\tag{E.1}
$$

with $\vec{\pi} = (\pi, \pi)$ the Brillouin vector. τ_1, τ_2 and τ_3 are Pauli matrices

$$
\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\tag{E.2}
$$

$f^{\dagger}_{1,\vec{k},\sigma}$ and $f_{1,\vec{k},\sigma}$ ($f^{\dagger}_{2,\vec{k},\sigma}$ and $f_{2,\vec{k},\sigma}$) are fermion creation and annihilation operators near the point $(\frac{\pi}{2}, \frac{\pi}{2})$ $((-\frac{\pi}{2}, \frac{\pi}{2}))$.
Rotating the operators

$$\begin{cases} f_{\vec{k}} = \frac{1}{\sqrt{2}}\left(f_{a,\vec{k}} + f_{b,\vec{k}}\right) \\ f_{\vec{k}+\vec{\pi}} = \frac{1}{\sqrt{2}}\left(f_{a,\vec{k}} - f_{b,\vec{k}}\right) \end{cases} \tag{E.3}$$

leads to

$$H = \sum_{\vec{k}\in SBZ}\sum_{\sigma}\psi^{\dagger}_{\vec{k}\sigma}\left[-\mu\mathbb{I} + \widetilde{\Delta}k_{+}\begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_2 \end{pmatrix} - \widetilde{\Delta}k_{-}\begin{pmatrix} \tau_2 & 0 \\ 0 & \tau_1 \end{pmatrix}\right]\psi_{\vec{k}\sigma} \tag{E.4}$$

where $k_+ = k_x + k_y$ and $k_- = k_x - k_y$, $\widetilde{\Delta} = 2\Delta\cos\frac{\pi}{4}$ and

$$\psi_{\vec{k}\sigma} = \begin{pmatrix} f_{1a,\vec{k}\sigma} \\ f_{1b,\vec{k}\sigma} \\ f_{2a\vec{k}\sigma} \\ f_{2b\vec{k}\sigma} \end{pmatrix} \tag{E.5}$$

In the Euclidean metric the action reads

$$\begin{aligned} S_E &= \int_0^{\tau} d\tau \sum_{\vec{k}\in SBZ}\sum_{\sigma}\psi^{\dagger}_{\vec{k}\sigma}\begin{pmatrix} \tau_3 & 0 \\ 0 & \tau_3 \end{pmatrix}\left[(\partial_\tau - \mu)\begin{pmatrix} \tau_3 & 0 \\ 0 & \tau_3 \end{pmatrix}\right. \\ &+ \left. i\widetilde{\Delta}k_{+}\begin{pmatrix} \tau_2 & 0 \\ 0 & -\tau_1 \end{pmatrix} + i\widetilde{\Delta}k_{-}\begin{pmatrix} \tau_1 & 0 \\ 0 & -\tau_2 \end{pmatrix}\right]\psi_{\vec{k}\sigma} \end{aligned} \tag{E.6}$$

Through the unitary transformation

$$\psi_{\vec{k}\sigma} \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}\tau_3} \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 \\ 0 & -\tau_1 \end{pmatrix}\psi_{\vec{k}\sigma} \tag{E.7}$$

and writing $k_+ = k_2$ and $k_- = k_1$

$$S_E = \int_0^{\beta} d\tau \sum_{\vec{k}\in SBZ}\sum_{\sigma}\bar{\psi}_{\vec{k}\sigma}\left[\gamma^0\left(\partial_\tau - \mu\right) + \widetilde{\Delta}ik_1\gamma^1 + \widetilde{\Delta}ik_2\gamma^2\right]\psi_{\vec{k}\sigma} \tag{E.8}$$

where $\bar{\psi} = \psi^{\dagger}\gamma^0$ and the γ matrices are defined as

$$\gamma^0 = \begin{pmatrix} \tau_3 & 0 \\ 0 & -\tau_3 \end{pmatrix},\ \gamma^1 = \begin{pmatrix} \tau_1 & 0 \\ 0 & -\tau_1 \end{pmatrix},\ \gamma^2 = \begin{pmatrix} \tau_2 & 0 \\ 0 & -\tau_2 \end{pmatrix} \tag{E.9}$$

Using the inverse Fourier transform $\psi_{\vec{k}\sigma} = \int d^2\vec{r}\psi_{\vec{r}\sigma}e^{i\vec{k}.\vec{r}}$ the Euclidean action reads finally

$$S_E = \int_0^{\beta} d\tau \int d^2\vec{r}\sum_{\sigma}\bar{\psi}_{\vec{r}\sigma}\left[\gamma^0\left(\partial_\tau - \mu\right) + \widetilde{\Delta}\gamma^k\partial_k\right]\psi_{\vec{r}\sigma} \tag{E.10}$$

With a "light velocity" $v_\mu = (1, \widetilde{\Delta}, \widetilde{\Delta})$ leading to a curved metric as explained in subsection 6.2.1.

E.2 Derivation of the photon polarization function at finite temperature

The Fourier transformation of the second term of the spinon action given by equation (6.15) reads

$$\begin{aligned} S_E^{(2)}[\psi,a] &= \sum_\sigma \sum_{\widetilde{\omega}_{F,1},\widetilde{\omega}_{F,2}} \int \frac{d^2\vec{k}_1}{(2\pi)^2} \int \frac{d^2\vec{k}_2}{(2\pi)^2} \bar{\psi}_\sigma(k_1) \\ & \left[\quad \frac{i\gamma^\mu k_\mu}{(2\pi)^2\beta}\delta(k_1-k_2) - \frac{ig\gamma^\mu a_\mu(k_1-k_2)}{(2\pi)^2\beta)^2} \right] \psi_\sigma(k_2) \end{aligned} \tag{E.11}$$

with $k = (\widetilde{\omega}_F \equiv \frac{2\pi}{\beta}(n+1/4),\vec{k})$. Integrating over the fermion field ψ and keeping the second order in the gauge field leads to the effective gauge action

$$S_{eff}^{(2)}[a] = \frac{1}{2} Tr\left[G_F.ig\gamma^\mu a_\mu\right]^2 \tag{E.12}$$

with $Tr = \sum\limits_{\omega_F^{'}} \int \frac{d^2\vec{k'}}{(2\pi)^2}.\sum\limits_{\omega_F^{''}} \int \frac{d^2\vec{k''}}{(2\pi)^2} tr$. The trace tr extends over the γ matrix space, and $G_F^{-1}(k_1-k_2) = i\frac{\gamma^\mu k_\mu}{(2\pi)^2\beta}\delta(k_1-k_2)$. The pure gauge action comes as

$$\begin{aligned} S_{eff}^{(2)}[a] &= -g^2\frac{1}{2\beta}\sum_\sigma\sum_{\omega_{F,1}}\int \frac{d^2\vec{k}_1}{(2\pi)^2}.\frac{1}{\beta}\sum_{\omega_F^{''}}\int \frac{d^2\vec{k''}}{(2\pi)^2} \\ & tr\left[\frac{\gamma^\rho k_{1,\rho}}{k_1^2}.\gamma^\mu a_\mu(k_1-k^{''}).\frac{\gamma^\eta k_\eta^{''}}{k^{''2}}.\gamma^\nu a_\nu\left(-(k_1-k^{''})\right)\right] \end{aligned} \tag{E.13}$$

With the change of variables $k_1 - k^{''} = q$ and $k_1 = k$

$$S_{eff}^{(2)} = -\frac{1}{2\beta}\sum_{\omega_B}\int \frac{d^2\vec{q}}{(2\pi)^2} a_\mu(-q)\Pi^{\mu\nu}(q)a_\nu(q). \tag{E.14}$$

where $q = (\omega_B = \frac{2\pi}{\beta}m, \vec{q})$ and the polarization function is given by

$$\Pi^{\mu\nu}(q) = \frac{g^2}{\beta}\sum_\sigma\sum_{\omega_F}\int \frac{d^2\vec{k}}{(2\pi)^2} tr\left[\frac{\gamma^\rho k_\rho}{k^2}.\gamma^\mu.\gamma^\eta\frac{(k_\eta+q_\eta)}{(k+q)}.\gamma^\nu\right] \tag{E.15}$$

Then using the Feynmann identity $\frac{1}{ab} = \int_0^1 dx \frac{1}{(ax+(1-x)b)^2}$ $\Pi^{\mu\nu}$ can be rewritten as

$$\Pi^{\mu\nu}(q) = \frac{g^2}{\beta}\sum_\sigma\sum_{\omega_F}\int \frac{d^2\vec{k}}{(2\pi)^2} tr\left[\gamma^\rho\gamma^\mu\gamma^\eta\gamma^\nu\right].\int_0^1 dx \frac{k_\rho(k_\eta+q_\eta)}{\left[(k+q)^2x+(1-x)k^2\right]^2} \tag{E.16}$$

By means of a change of variables $k \rightarrow k^{'} - xq$ and using the identity $tr\left[\gamma^{\rho}\gamma^{\mu}\gamma^{\eta}\gamma^{\nu}\right] = 4.\left[\delta_{\rho\mu}.\delta_{\eta\nu} - \delta_{\rho\eta}.\delta_{\mu\nu} + \delta_{\rho\nu}.\delta_{\mu\eta}\right]$ one obtains

$$\begin{aligned}
\Pi^{\mu\nu}(q) &= 4\alpha \int_0^1 dx \frac{1}{\beta}\sum_{\omega_F^{'}} \int \frac{d^2\vec{k'}}{(2\pi)^2}\Bigg\{ \Big[2k_{\mu}^{'}k_{\nu}^{'} \\
&+ (1-2x)(k_{\mu}^{'}q_{\nu} + q_{\mu}k_{\nu}^{'}) - x(1-x)2q_{\mu}q_{\nu} \\
&- \delta_{\mu\nu}\sum_{\eta}\left({k_{\eta}^{'}}^2 + (1-2x)k_{\eta}^{'}q_{\eta} - x(1-x){q_{\eta}}^2 \right) \\
&\quad \Big] / \left[{k^{'}}^2 + x(1-x)q^2 \right]^2 \Bigg\}
\end{aligned} \tag{E.17}$$

where $\alpha = g^2 \sum_{\sigma=1}^{N=2} 1$. Following Dorey and Mavromatos [24], Lee [48], Aitchison *et al.* [3] and Gradshteyn [30] we define

$$\begin{aligned}
S_1 &= \sum_{n=-\infty}^{\infty} \frac{1}{\left[{k'}^2 + x(1-x)q^2 \right]} \\
&= \frac{\beta^2}{4\pi Y}\left[\frac{\sinh(2\pi Y)}{\cosh(2\pi Y) - \cos(2\pi X)} \right]
\end{aligned} \tag{E.18}$$

$$S_2 = \sum_{n=-\infty}^{\infty} \frac{1}{\left[{k'}^2 + x(1-x)q^2 \right]^2} = -\frac{\beta^2}{8\pi^2}.\frac{1}{Y}\frac{\partial S_1}{\partial Y} \tag{E.19}$$

$$S^{*} = \sum_{n=-\infty}^{\infty} \frac{\omega_F^{'}}{\left[{k'}^2 + x(1-x)q^2 \right]^2} = -\frac{\beta}{4\pi}\frac{\partial S_1}{\partial X} \tag{E.20}$$

with $X = x.m + 1/4$ and $Y = \frac{\beta}{2\pi}\sqrt{\vec{k'}^2 + x(1-x)q^2}$. The polarization can be expressed in terms of these sums and reads

$$\begin{aligned}
\Pi^{00} &= \frac{\alpha}{\beta}\int_0^1 dx \int \frac{d^2\vec{k'}}{(2\pi)^2}\Big[S_1 - 2\left[\vec{k'}^2 + x(1-x)q_0^2 \right] S_2 \\
&+ (1-2x)q_0 S^{*} \Big]
\end{aligned} \tag{E.21}$$

for the temporal component and

$$\begin{aligned}
\Pi^{ij} &= \frac{\alpha}{\beta}\int_0^1 dx \int \frac{d^2\vec{k'}}{(2\pi)^2}\Big[2x(1-x)(q^2\delta_{ij} - q_i q_j)S_2 \\
&- (1-2x)q_0\delta_{ij}.S^{*} \Big]
\end{aligned} \tag{E.22}$$

for the spatial components.

Integrating over the fermion momentum $\vec{k'}$ one gets

$$\Pi^{00} = \widetilde{\Pi}_3 - \frac{q_0^2}{q^2}\widetilde{\Pi}_1 - \widetilde{\Pi}_2 \tag{E.23}$$

$$\Pi^{ij} = \widetilde{\Pi}_1 \left(\delta_{ij} - \frac{q_i q_j}{q^2}\right) + \widetilde{\Pi}_2 \delta_{ij} \tag{E.24}$$

where

$$\widetilde{\Pi}_1 = \frac{\alpha q}{\pi} \int_0^1 dx \sqrt{x(1-x)} \frac{\sinh \beta q \sqrt{x(1-x)}}{D(X,Y)} \tag{E.25}$$

$$\widetilde{\Pi}_2 = \frac{\alpha m}{\beta} \int_0^1 dx (1-2x) \frac{\cos 2\pi x m}{D(X,Y)} \tag{E.26}$$

$$\widetilde{\Pi}_3 = \frac{\alpha}{\pi\beta} \int_0^1 dx \ln 2D(X,Y) \tag{E.27}$$

and $D(X,Y) = \cosh\left(\beta q\sqrt{x(1-x)}\right) + \sin(2\pi x m)$.

List of Figures

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