ISAS - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES

Ground State of the U infinite Hubbard Model in two Dimensions

Thesis submitted for the degree of

"Magister Philosophiæ"

CANDIDATE

Michela Di Stasio

SUPERVISORS

Prof. Giuseppe Morandi

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October 1991

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SISSA - SCUOLA INTERNAZIONALE SUPERIORE I STUDI AVANZATI

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1 Introduction

The discovery of superconductivity in the Copper-Oxides compounds [1] and the Anderson's suggestion [3] of the relevance of the large U limit of the Hubbard model has triggered a renewed interest in this model and more in general in strongly correlated electron systems.

The Hubbard model,proposed in 1964 by Hubbard himself [2], stimulated the search for a variety of approximate and exact techniques to understand its behaviour. However, only the one dimensional case is by now well understood due to the existence of an exact Bethe ansatz solution, and to the possibility of applying well-known field theory techniques such as renormalization group techniques and bosonization method to study it.

The Hubbard model contains two contrary playing terms: the kinetic one, which tends to delocalize electrons in bands, and the Coulomb repulsion that favors localization of electrons. Approximate treatments succeded in describing the so called Mott-Hubbard insulators and the charge-transfer insulators [5].

Whether the essential properties of the Copper Oxygen planes in the High T_c superconductors could be described by a two dimensional extended Hubbard model or not is still a matter of debate [4]. For the two-band Hubbard model with Coulomb repulsion only in

the Copper sites a single band effective Hamiltonian was derived [8]: the t-J Hamiltonian.

Of particular relevance in order to understand HTCS are the following questions:

What are the phases of the extended Hubbard model?

Does the ground state exhibit long-range spin order?

What are the low-energy excitations?

Can superconductivity occur?

The answers to these questions for the strong repulsive case are still lacking. As fully interacting many-body systems, neither the Hubbard nor the Heisenberg Hamiltonian can be treated by standard many-body perturbation theory, since no small parameters are present.

We are concerned here with the Hubbard Hamiltonian at half filling (one electron per site) on a square lattice and in the limit $U \to \infty$, i.e. the Heisenberg Hamiltonian acting on the restricted Hilbert space, with single site occupancy. It should also be said that a careful study of the 2D Hubbard model at half filling and in the strong coupling limit can possibly yield some insights into the highly non trivial dynamics of a 2D quantum Heisenberg antiferromagnet.

A brief introduction to the Hubbard Hamiltonian, the large U expansion and the tentative phase diagram will be discussed in the next chapter (chapter 2 "From Hubbard to t-J model"). There we also address the still open question of whether, at half filling, long range Neel order ([6],[13],[15]) occurs or other phases, suggested by mean field theory ([16],[10],[17]), are present.

The original part of this thesis consists in the presentation of an exact method to implement the constraint of no double-occupancy of sites ($U \to \infty$), at half filling and at

finite temperature (chapter 3 "Path integral expression for the partition function in the restricted subspace").

The most popular approach to the ground state of the Heisenberg model at half filling (symmetry group $SU(N), N = 2$) is the saddle point approximation to evaluate the path integral expression of the partition function. The result becomes exact for its generalization to $SU(N)$ antiferromagnets in the limit N going to infinity.

The large N expansion consists of enlarging the symmetry group from SU(2) to SU(N). This is very different from changing the representation from $S = 1/2$ to larger values of S, which tends to the classical limit. It is also possible to calculate the corrections in $1/N$.

An auxiliary field is introduced in the $N-$component Lagrangian to account for the average site occupancy of $N/2$. The large N limit quenches the fluctuations of this occupation number regardless of the value of U (U $>$ 0)[7]. This also happens when the constraint is handled within the slave boson method [18].

At finite N the infinite U limit should completely suppress the fluctuations which could possibly arise. However this feature is hard to reproduce.

Numerical methods are being developed ([9],[11], [12]), while the slave boson technique is expected not to give reliable results at finite temperature.

At zero temperature, the constraint of single site occupancy (U $\rightarrow \infty, N = 2$) has been implemented in recent calculations by means of the Gutzwiller projection, and the resulting ground state has been found to have good variational energy [14].

Our work originates from the observation that, when $N = 2$, the constraint of half filling takes a very simple form and can be implemented exactly at any temperature.

Therefore, the compromise choice we have made was to project properly onto the restricted subspace when evaluating the fermion trace with $N = 2$ and to perform the saddle point approximation, with no pretention of it being exact in some limit.

The classical theorem[42] in path integral theory, saying that the saddle point approximation gives the same free energy which one would obtain from an Hartree–Fock approximation on an original Hamiltonian, doesn't hold for constrained path integrals and this is explicitly our case.

The Hubbard-Stratonovich decoupling of the fermion interaction term introduces an auxiliary boson field. We study two generalized mean field solutions (dimer phase and flux phase, both of periodicity $\sqrt{2}\mathrm{X}\sqrt{2}$) which are the ones first discovered by Affleck and Marston[16] (AM). (chapter 4 "Static approximations and saddle point solutions"). We will not consider, for example, the so called columnar dimer phase (2X1 unit cell) which has been found[23] to be stabilized by quantum fluctuations against the so called staggered dimer phase which we are dealing with. Also the Flux phase has been found to be unstable with respect to a box phase[24] (2X2 unit cell) but it could be stabilized by adding further interactions[7]. (See the next chapter for other possible phases).

These phases are still stationary points of the action also in presence of the constraint. The latter has the role of inhibiting classical fluctuations and this will cause an increase of the mean field transition temperature.

The static gaussian fluctuations around these saddle points give us informations about the stability of the phases and the collective excitations. (chapter 5 "Gaussian fluctuations"). We will consider only gaussian fluctuations with the same space periodicity as the mean field solutions ($\sqrt{2}\mathrm{X}\sqrt{2}$ unit cell). The U(1) symmetry of the action also implies

the appearence of zero modes which have been identified.

Next we have studied the effect of the constraint on the free energy at any temperature within the saddle point approximation. The inclusion of the constraint acts as an effective reduction of the entropy of the system at finite temperature. As a consequence the action calculated at the saddle point shows the wrong temperature dependence because it is incresing with temperature, so that it cannot be assumed as an approximation to the free energy. Therefore, in evaluationg the free energy, we have to include the gaussian fluctuations (one loop corrections) previously examined taking care of the zero modes. (chapter 6 "Free energy including gaussian fluctuations"). Because only static fluctuations are considered our extimate of the free energy can be viewed as an approximation valid at intermediate temperatures. The free energy of the flux phase we obtain is higher than that of Peierls dimer phase, which again results as the most stable one.

In the last chapter of this thesis we sketch the way how our method could be extended away from half filling. (chapter 7 "Extension away from half filling"). In this case the full Gutzwiller projector has to be included to garantee no double occupancy of sites. Because it does not commute with the t-J Hamiltonian the extension of this method away from half filling is not trivial at all.

2 From Hubbard to t-J model

This chapter is intended to provide a general framework to our work. A brief introduction to the Hubbard model and to its large U expansion is given stressing the peculiarity of the half-filling case. A great variety of possibly occurring ground states has been proposed. Here we will focus our attention on the dimerized Peierls phases and on the flux phases in order to better clarify their origins and some of the still open questions.

The Hubbard model describes fermions with only one orbital degree of freedom and spin 1/2, when the on−site Coulomb interaction, in a tight binding description, is dominant. The Hubbard Hamiltonian reads:

$$H = t \sum_{<i,j>,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma}) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \tag{2.1}$$

where $c^{\dagger}_{i,\sigma}$ creates a fermion at site i with spin $\sigma = \uparrow, \downarrow$; t is the nearest-neighbour hopping matrix element and $U > 0$ is the on-site Coulomb repulsion.

Recently Yang et al. [28] showed that the Hubbard Hamiltonian has a SO(4) symmetry in the spin and pseudo-spin space. They were able to classify exactly all the eigenstates of the Hubbard model. Except for this exact result we don't know what type and in what parameter regime a broken symmetry state may be stable.

The first term in equation (2.1) corresponds, for a square lattice with lattice spacing $a = 1$, to an energy band $\epsilon(\vec{k}) = -2t(cos(k_x) + cos(k_y))$. A very important peculiarity of the half-filled (n =1) case is the perfect nesting of the Fermi surface; i.e., the Fermi surface is invariant with respect to a translation by a vector $\vec{Q} = (\pi, \pi)$. Therefore, for n = 1, the system is subject to an antiferromagnetic instability for arbitrary small values of U. A gap will open $\forall$ U/t at T = 0 and the system will be an insulator. For a more general $\epsilon(\vec{k})$ the system will remain metallic for small U. But for $U > U_c$ a transition to a Mott insulator is expected. In magnetically non frustrated systems, this transition should be accompanied by antiferromagnetic ordering. In frustrated systems (either by lattice effects or competing interactions) this transition could be from paramagnetic metal to paramagnetic insulator.

What happens when U is large ?

Clearly doubly-occupied sites are energetically very unfavorable, and will be present in the low energy spectrum only virtually. However, to have finite values of t/U, we must incorporate the effects of the virtual processes which connect the reduced Hilbert space (no doubly-occupied sites) to larger spaces with doubly occupied sites.

An unitary transformation e^{iS} on the Hilbert space can be performed in order to eliminate high energy processes in lowest order t/U. Such a procedure has a long history going back to the early work of Kohn [26] (1964). Since we are especially interested in the behaviour at or near half-filling we can neglect the so called three-site hopping contribution. At first order in t/U we get the $t - J$ Hamiltonian:

$$H_{tJ} = \mathcal{P}(-t \sum_{<i,j>,\sigma} (d^{\dagger}_{i,\sigma} d_{j,\sigma} + d^{\dagger}_{j,\sigma} d_{i,\sigma})\mathcal{P} + J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \qquad (2.2)$$

where $J = 4t^2/U$ and $\mathcal{P} = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$ is the Gutzwiller projector. This effective Hamiltonian is valid only in the subspace with no doubly-occupied sites, since it corresponds to the first term of a perturbation expansion in t/U in this subspace. For $U = \infty$ only the kinetic term survives, and for exactly one hole Nagaoka [25] showed that the system is ferromagnetically ordered.

We mostly discuss the case of half filling in what follows. At half filling the kinetic energy term exactly vanishes, so that we have a Heisenberg Hamiltonian acting inside a spin-only subspace.

Generalizations of the Heisenberg model $SU(2)$ for fermions with spin $1/2$ to $SU(N)$ antiferromagnets with $n_c = 2S$ particle's colors were introduced in the past. This allows to study very different limits as $n_c \to \infty$ and $N \to \infty$. In the former case it has been proved [43] that the lowest energy state is a Neel state, i.e. it has long range antiferromagnetic correlations. In this limit, in fact, one moves towards the classical limit. A completely different physics is given by the large N limit. In this case, the saddle point evaluation of the partition function becomes exact. Many dimerized spin-Peierls phases have been found to be degenerate and to have lower free energy with respect to the Neel state. When including $1/N$ corrections one can show [23] that a columnar arrangement of dimers gains energy from special fluctuations. However, the outcoming phase diagram S *vs.* N leaves the case $S = 1/2$, $N = 2$ uncertain.

It is easy to see that the Heisenberg Hamiltonian is locally gauge invariant under a SU(2) gauge transformation:

$$d^\dagger_{i,\uparrow} \quad \to \quad \alpha_i d^\dagger_{i,\uparrow} + \beta_i d_{i,\downarrow}$$

$$d_{i,\downarrow} \rightarrow -\beta_i^{\star} d_{i,\uparrow}^{\dagger} + \alpha_i^{\star} d_{i,\downarrow} \tag{2.3}$$

where $\mid \alpha_i \mid^2 + \mid \beta_i \mid^2 = 1$.

A wide class of possibilities arises depending on the choice of order parameters ([27],[9]) used to build up a self consistent mean field theory.

Variational approaches have also been adopted. The proposed "projected wave functions" are of the form:

$$\mid \Phi > = \mathcal{P} \mid \Phi_{HFB} > \tag{2.4}$$

where the Hartree-Fock-Bogoliubov wave function $\mid \Phi_{HFB} >$ can be a Fermi liquid ($\mid \Phi_{FL} >$), a spin density wave ($\mid \Phi_{SDW} >$), a Bardeen-Cooper-Schrieffer ($\mid \Phi_{BCS} >$ wave function or a combination of these.

Consider, for example, the BCS case:

$$\mid \Phi_{HFB} > = \mid \Phi_{BCS} > = \prod_k (u_k + v_k d_{k,\uparrow}^{\dagger} d_{-k,\downarrow}^{\dagger}) \tag{2.5}$$

In the most general case, in evaluating the mean field expectation values we must include both types of averages:

$$\begin{aligned} \Delta_r &= < d_{i,\uparrow}^{\dagger} d_{i+r,\downarrow}^{\dagger} - d_{i+r,\uparrow}^{\dagger} d_{i,\downarrow}^{\dagger} > \\ \xi_r &= \sum_{\sigma} < d_{i,\sigma}^{\dagger} d_{i+r,\sigma} > \end{aligned} \tag{2.6}$$

where $r = x, y$ and $i + r$ denotes the nearest neighbour of i in the r direction.

Zhang et al.[30] and Kotliar et al.[18] found that there are many different choises of Δ_r and ξ_r which lead to the same quasiparticle excitations spectrum. The explanation

for this large degeneracy in the choice of the fermion state $\mid \Phi_{HFB} >$, is the local SU(2) gauge symmetry of the Heisenberg Hamiltonian when represented in fermion operators.

(A single spin state, which satisfy the projection condition exactly, can be written in fermion language ($\mathcal{P} \mid \Phi >$) in very many ways. This very large redundancy in the fermion language results in a very large class of apparent degeneracies in the mean field theory.)

Affleck and Marston[16], and Kotliar[10] found different types of fermion states which have the same quasiparticle spectrum:

$$E(k) = \pm C\sqrt{\cos^2 k_x + \cos^2 k_y} \tag{2.7}$$

They called it a flux state and a (s + id)-wave RVB state respectively. The AM state is a form of Hartree-Fock state based on a Slater determinant made up of eigenfunctions for a single particle moving in a magnetic flux. The choice of an uniform magnetic flux equal to 1/2 the flux quantum $\left(\frac{hc}{e}\right)$ per plaquette leads to the Hartree-Fock Hamiltonian:

$$H = \sum_{<i,j>;\sigma} \left(e^{i\theta_{ij}} d^{\dagger}_{i,\sigma} d_{j,\sigma} + h.c. \right) \tag{2.8}$$

While the individual phases θ_{ji} do not have physical meaning, due to the possibility of gauge transformation, the total plaquette phase ($\sum_{\square} \theta_{ij} = \pi$) is a gauge invariant object which characterizes the state.

From variational Monte Carlo studies[35], the flux state turns out to be a paramagnetic state with very short range antiferromagnetic order. Recent numerical studies[31] seem to give good evidence of long range antiferromagnetic order for the ground state of the Heisenberg model. Up to now the lowest energy found in numerical studies ([33], [34]) corresponds to a state that combines RVB correlations and antiferromagnetic long range

order.

This is an overview of the situation at half filling.

Away from half filling antiferromagnetic order is unlikely and the flux state may be a good starting point to describe a paramagnetic state at finite doping. This would be unstable against antiferromagnetic order in absence of doping[32]. (A different kind of instability, namely towards a box phase, was found by Dombre and Kotliar[24], however Marston and Affleck[7] argue that this is no more the case when adding further interactions.)

The flux phase is particularly relevant because of gapless particle-hole excitations at special points of the Brillouin Zone with linear dispersion, giving rise to an approximate 2+1 dimensional (massless) relativistic free fermion quantum field theory. This could be the starting point[19] (by inclusion of frustration) for the so called "anyon superconductivity"[20].

In the doped case, H_{tJ} is no longer gauge invariant due to the kinetic energy term. The value of this last term, in the flux phases, depends on the gauge used to represent the flux. The best choice turns out to be that of the commensurate flux phases. These are obtained keeping the flux constant in each plaquette and then varying its magnitude in such a way that it is commensurate with the density ([36],[38]): $\theta = \sum_{\Box} \theta_{ij} = \pi(1-\delta)$.

There are however still open questions both from the experimental and the theoretical point of view. In this flux phases, at finite doping, there is a breaking of time reversal symmetry but experimental evidence, for or against this, is still lacking. From a theoretical point of view, still open questions concern the electromagnetic response[39] and the possible superconducting properties of these states. These difficulties arise, even at the RPA

level, due to the very peculiar energy spectrum of non interacting fermions in a 2-d lattice, when one introduces a flux in the kinetic energy; i.e.: the Hofstadter spectrum[37]. This is a complex fractal pattern which arises from the interference of lattice periodicity with that determined by the flux. Then, the problem of the electromagnetic response is related to the dynamical properties of a "quantum fractal system". Also for the superconducting properties, while the simpler description which ignores the complications of the lattice favours superconductivity, it is not clear if this survives in a realistic description[40].

3 Path integral expression for the partition function in the restricted subspace

In this chapter we set up a way of incorporating the constraint represented by the half filling projector into the Path Integral description of the partition function for the Heisenberg model. We are dealing with a two dimensional square lattice at half filling.

The Heisenberg Hamiltonian reads:

$$H = -\sum_{(i,j)} J_{ij} \vec{S}_i \cdot \vec{S}_j \tag{3.1}$$

or, expressing the spin operators in terms of the Fermion operators as:

$$\vec{S}_i = c^{\dagger}_{i,\alpha} \vec{\sigma}_{\alpha,\beta} c_{i,\beta} \tag{3.2}$$

where the $\sigma_{\alpha,\beta}$ are the elements of the Pauli matrices $\sigma^{1,2,3}$,

$$= -\frac{1}{2} \sum_{(i,j)} J_{ij} c^{\dagger}_{i,\alpha} c_{i,\beta} c^{\dagger}_{j,\beta} c_{j,\alpha} - \frac{1}{4} \sum_{(i,j)} J_{ij} (n_{i,\uparrow} - n_{i,\downarrow})(n_{j,\uparrow} - n_{j,\downarrow}) \tag{3.3}$$

This Hamiltonian can be rewritten in terms of the transfer operators defined by:

$$\chi_{ij} = \sum_{\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} \tag{3.4}$$

where $\chi_{ij} = \chi^{\dagger}_{ji}$ and $\chi_{ii} = n_i = n_{i,\downarrow} + n_{i,\uparrow}$ as:

$$H = -\frac{1}{2} \sum_{(i,j)} J_{ij} \chi^{\dagger}_{ij} \chi_{ij} \tag{3.5}$$

Here we have neglected additive terms which depend only on the occupation number operators n_i and are constant at half filling. We will consider here $J_{ij} = J$ for i,j nearest neighbours and 0 otherwise. To fix further the notation we will denote by $\sum_{(i,j)}$ the sum over ordered nearest neighbour pairs. The peculiarity of the half filling case is that the occupation number operator and the Hamiltonian commute:

$$[n_i, \chi^{\dagger}_{hk} \chi_{hk}] = 0 \qquad\qquad \forall i, h, k \tag{3.6}$$

Because we want to evaluate the partition function of the model at half filling, the particle number is fixed, so that the Canonical ensemble will be adopted. The partition function in the set of states in which site occupancy is one is:

$$\mathcal{Z} = Tr\{\mathcal{P} exp(-\beta H_o)\mathcal{P}\} = Tr\{exp(-\beta H_o)\mathcal{P}\} \tag{3.7}$$

where the single occupancy projector is given by $\mathcal{P} = \prod_i n_i(2 - n_i)$ and the ciclic properties of the trace have been used together with the properties of the projector $\mathcal{P}^2 = \mathcal{P}$.

Define now a new Hamiltonian:

$$H = H_o - \frac{1}{\beta} \sum_i z_i n_i \tag{3.8}$$

where, for the time being, the z_i's are taken as arbitrary real parameters. In terms of H we can build up the following generating function:

$$\mathcal{Z}[z] = Tr\{exp(-\beta H)\} \tag{3.9}$$

The original partition function can be easily obtained performing partial derivatives of this new function :

$$\mathcal{Z} = \prod_i \frac{\partial}{\partial z_i}(2 - \frac{\partial}{\partial z_i})\mathcal{Z}[z]\Big|_{z=0} \tag{3.10}$$

Partial derivatives with respect to z_i's are non ambiguous because n_i and H_0 commute.

For a lattice with N sites the Hilbert space of states contains altogether 4^N states, while the subspace of half filled states spans half of the Hilbert space, i.e. a manifold of states of dimension 2^N. Correspondingly, for $J = 0$, we obtain from eq. 3.7:

$$\mathcal{Z} \mid_{J=0} = Tr\{\mathcal{P}\} = 2^N \tag{3.11}$$

This implies of course that, in the limit $J = 0$, the only contribution to the Free Energy comes from the configurational Entropy, which is $Nk_B \ln 2$ for the half filled subspace, where k_B denotes the Boltzmann constant. It would be $Nk_B \ln 4$ for the whole Hilbert space, i.e. in the absence of the constraint.

It is standard procedure to express the generating function $\mathcal{Z}[z]$ as a Path Integral over Grassmann variables[41]:

$$\mathcal{Z}[z] = \int \prod_{i,\alpha} \mathcal{D}\psi^{\star}_{i,\alpha} \mathcal{D}\psi_{i,\alpha} \exp\left\{ - \int_0^1 d\tau \sum_{i,\alpha} \psi^{\star}_{i,\alpha}(\tau)(\partial_\tau - z_i)\psi_{i,\alpha} + \right.$$
$$\left. + \frac{\beta J}{2} \sum_{(i,j)} \sum_{\alpha,\beta} \int_0^1 d\tau \psi^{\star}_{i,\alpha}(\tau)\psi^{\star}_{j,\beta}(\tau)\psi_{i,\beta}(\tau)\psi_{j,\alpha}(\tau) \right\} \tag{3.12}$$

Here τ is a scaled imaginary time variable ranging from 0 to 1, the ψ's and $\psi^{\star}$'s are Grassmann variables obeying antiperiodic boundary conditions in τ at the extremes of the interaval $[0,1]$, and the symbols $\mathcal{D}\psi^{\star}_{i,\alpha}$ and $\mathcal{D}\psi_{i,\alpha}$ stand for the path integration over the Grassmann variables.

We introduce next the Hubbard Stratonovich fields:

$$\mathcal{U}_{ij}(\tau) = \sum_{\beta} \psi^{\star}_{i,\beta}(\tau)\psi_{i,\beta}(\tau) \tag{3.13}$$

And use the identity:

$$\exp\left\{ \frac{\beta J}{2} \sum_{\alpha,\beta} \int_0^1 d\tau \psi^{\star}_{i,\alpha}(\tau)\psi^{\star}_{i,\beta}(\tau)\psi_{j,\beta}(\tau)\psi_{j,\alpha}(\tau) \right\} =$$
$$\int \mathcal{D}\mathcal{U}_{ij} \exp\left\{ -\pi \int_0^1 d\tau \left(\mid \mathcal{U}_{ij}(\tau) \mid^2 - \sqrt{\frac{\pi\beta J}{2}} \sum_{\alpha} (\psi^{\star}_{i,\alpha}(\tau)\mathcal{U}_{ij}(\tau)\psi_{j,\alpha}(\tau) + c.c.) \right) \right\} \tag{3.14}$$

where the symbol $\int \mathcal{D}\mathcal{U}_{ij}$ represents the integrals over the Real and Imaginary parts of the auxiliary boson fields $\mathcal{U}_{ij}$: $\int d\Re\{\mathcal{U}_{ij}\} d\Im\{\mathcal{U}_{ij}\}$.

Note that the $\mathcal{U}$'s obey periodic boundary conditions in τ, and satisfy moreover:

$$\mathcal{U}^{\star}_{ij}(\tau) = \mathcal{U}_{ji}(\tau) \tag{3.15}$$

This means that if we consider $\mathcal{U}$ as a matrix in the site indices, $\mathcal{U}$ is an Hermitian matrix:

$$\mathcal{U}^{\dagger}(\tau) = \mathcal{U}(\tau) \qquad ; \qquad \tau \in [0,1] \tag{3.16}$$

It is useful to introduce the Fourier transforms of the various fields, i.e.:

$$\begin{aligned} \psi_{i,\alpha}(\tau) &= \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} \psi_{i,\alpha}(\omega_n) \\ \mathcal{U}_{ij} &= \sum_{m=-\infty}^{\infty} e^{-i\Omega_m \tau} \mathcal{U}_{ij}(\Omega_m) \end{aligned} \tag{3.17}$$

where on account of the boundary conditions:

$$\omega_n = (2n+1)\pi \qquad ; \qquad \Omega_m = 2m\pi \tag{3.18}$$

that are the Matsubara frequencies for fermionic and bosonic fields respectively. Note that the hermiticity condition on $\mathcal{U}(\tau)$ reads now:

$$\mathcal{U}_{ij}(\Omega_m) = \mathcal{U}^{\star}_{ji}(-\Omega_m) \tag{3.19}$$

Finally performing the Hubbard Stratonovich transformation, moving to Fourier space and using the definition of the Kroenecker delta:

$$\delta_{\omega_n,\omega_{n'}} = \int_0^1 d\tau e^{-i(\omega_n - \omega_{n'})\tau} \tag{3.20}$$

we find that the generating function is given by:

$$\mathcal{Z}[z] = \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} \prod_{i,\alpha} \mathcal{D}\psi^{\star}_{i,\alpha} \mathcal{D}\psi_{i,\alpha} exp\{-\pi \sum_{(i,j)} \sum_{m} \mid \mathcal{U}_{ij}(\Omega_m) \mid^2 + \\ + \sum_{(i,j)} \sum_{\alpha} \sum_{n,n'} \psi^{\star}_{i,\alpha}(\omega_n) A^{nn'}_{ij} \psi_{j,\alpha}(\omega'_n) + c.c.)\} \tag{3.21}$$

where:

$$A^{nn'}_{ij} = (i\omega_n + z_i)\delta_{i,j}\delta_{n,n'} - c\, \mathcal{U}_{ij}(\omega_n - \omega'_n) \tag{3.22}$$

and $c = \sqrt{\pi\beta J/2}$.

Note that $\mathcal{U}^{n,n'}_{ij}$ is hermitian when considered as a matrix in the site and the fermion frequency indices:

$$\mathcal{U}^{n,n'}_{ij} = (\mathcal{U}^{n',n}_{ji})^{\star} \tag{3.23}$$

Now the integration over Grassmann variables is standard, since we have a quadratic form in the ψ fields, and yields:

$$\mathcal{Z}[z] = \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} \exp\{-\pi \sum_{(i,j)} \sum_{m} \mid \mathcal{U}_{ij}(\Omega_m) \mid^2 + 2Tr \ln A\} \tag{3.24}$$

where the factor 2 comes from the summation over spin indices.

This result can be rewritten in terms of the single particle Green's function G_o, for J=0, whose matrix elements are:

$$(G_o)^{n,n'}_{ij} = \frac{1}{i\omega_n}\delta_{i,j}\delta_{n,n'} \tag{3.25}$$

that is antihermitian, and of the matrix:

$$(\tilde{\mathcal{U}})_{ij}^{n,n'} = z_i \delta_{i,j} \delta_{n,n'} - c\mathcal{U}_{ij}(\omega_n - \omega_{n'}). \tag{3.26}$$

We get:

$$\mathcal{Z}[z] = \mathcal{N} \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} \exp\{-\pi \sum_{(i,j)} \sum_{m} \mid \mathcal{U}_{ij}(\Omega_m) \mid^2 + 2Tr \ln[1 + G_o \tilde{\mathcal{U}}]\} \tag{3.27}$$

The normalization factor is $\mathcal{N} = \exp[2Tr \ln G_o^{-1}] = 4^N$ when evaluated using standard contour−integral techniques.

An effective Action can be introduced:

$$S_{eff}[\tilde{\mathcal{U}}] = -2Tr \ln[1 + G_o \tilde{\mathcal{U}}] \tag{3.28}$$

At this stage we can take the appropriate derivatives with respect to the z_i's and set $z_i = 0$ to obtain the partition function at half-filling.

According to the equation (3.10) the partition function becomes:

$$\mathcal{Z} = \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} \exp\left\{-\pi \sum_{(i,j)} \sum_{m} \mid \mathcal{U}_{ij}(\Omega_m) \mid^2 - S_{eff}[c\mathcal{U}] + \sum_i \ln 4B_i[\mathcal{U}]\right\} \tag{3.29}$$

where the last term arises from the constraint of half-filling, with:

$$B_i[\mathcal{U}] = \left(\frac{\partial^2 S_{eff}[\mathcal{U}]}{\partial z_i^2} - 2\frac{\partial S_{eff}[\mathcal{U}]}{\partial z_i} - \left(\frac{\partial S_{eff}[\mathcal{U}]}{\partial z_i}\right)^2\right)\Bigg|_{z=0} \tag{3.30}$$

Differentiating with respect to z_i and exploiting the cyclic invariance of the trace, we find:

$$\frac{\partial S_{eff}[\tilde{\mathcal{U}}]}{\partial z_i} = -2Tr\left\{(1 - cG_o\tilde{\mathcal{U}})^{-1} G_o P_i\right\} \tag{3.31}$$

From the point of view of site indices, taking traces of powers of $\mathcal{U}$ correspond to building up loops of appropriate length in the lattice. If we specialize our results to the case of a square lattice and of nearest neighbour couplings, it is not difficult to convince oneself that only loops with an even number of sites will be allowed, and hence only even powers of $\mathcal{U}$ will survive the trace operation. In this case, the first variation of the effective action is:

$$\left.\frac{\partial S_{eff}[\mathcal{U}]}{\partial z_i}\right|_{z=0} = -1 - 2Tr\left\{\frac{c^2(G_o\mathcal{U})^2}{1-c^2(G_o\mathcal{U})^2}G_oP_i\right\} \tag{3.32}$$

In the Wannier rapresentation, P_i is the projector to the Wannier function localized on the $i-th$ site of the lattice, so that $(P_i)_{jk} = \delta_{jk}\delta_{ij}$.

The second derivative of S_{eff} can be evaluated along lines similar to those leading to (3.32). The result is:

$$\begin{aligned}\left.(\frac{\partial^2 S_{eff}}{\partial z_i^2})\right|_{z=0} &= 2Tr\left\{\left[(1-cG_o\mathcal{U})^{-1}G_oP_i\right]\right\} \\ &= 2Tr\left\{\left[(1-c^2(G_o\mathcal{U})^2)^{-1}G_oP_i\right]^2\right\}\end{aligned} \tag{3.33}$$

The partition function can be rewritten as:

$$\mathcal{Z} = \int \prod_{(i,j)} \mathcal{D}\mathcal{U}_{ij} exp\{-\beta\mathcal{F}_{eff}[\mathcal{U}]\} \tag{3.34}$$

where an effective free energy is introduced:

$$\beta\mathcal{F}_{eff}[\mathcal{U}] = \pi\sum_{(i,j)}\sum_m \mid \mathcal{U}_{ij}^m \mid^2 + S_{eff}[c\mathcal{U}] - \sum_i \ln 4B_i[\mathcal{U}] \tag{3.35}$$

The constraint acts as a term which reduces the entropy. In fact we shall find that B_i is larger than $1/2$ in the static approximation to be discussed in the next chapter.

4 Static Approximation and Saddle Point Solutions

Having set up the general formalism in the previous chapter we discuss now the static approximation for the Path Integral. This amounts to restricting the integral to paths that are constant in "time", i.e. that satisfy:

$$\mathcal{U}_{ij}^{n,n'} = \mathcal{U}_{ij}\delta_{n,n'} \tag{4.1}$$

where the matrix $\mathcal{U}$ is now hermitian in the site indices. The static approximation brings about a great simplification of the formalism since all the frequency sums decouple from those over site indices.

The explicit expression for S_{eff} is given by the series:

$$S_{eff}[\tilde{\mathcal{U}}] = 2\sum_{k=1}^{\infty}\frac{(-1)^k}{k}Tr\{(G_o\tilde{\mathcal{U}})^k\} = -\sum_{i=1}^{N}z_i + 2\sum_{k=2}^{\infty}\frac{(-1)^k}{k}\chi_k Sp[(\tilde{\mathcal{U}})^k] \tag{4.2}$$

where $\chi_k = \sum_n(\frac{1}{i\omega_n})^k$ and $\chi_{2k+1} = 0$ and the symbol "Sp" indicates the trace over site indices alone.

Its first derivative with respect to z_i reads:

$$\frac{\partial S_{eff}[\tilde{\mathcal{U}}]}{\partial z_i} = -1 + \sum_{k=1}^{\infty}2\chi_{2k}Sp[\tilde{\mathcal{U}}^{2k}\tilde{\mathcal{U}}^{-1}P_i] \tag{4.3}$$

For a square lattice and only nearest neighbour interactions $\frac{\partial S_{eff}}{\partial z_i}\Big|_{z=0} = -1$. In fact the trace over site indices of powers of the auxiliary bosonic fields corresponds to building up loops of appropriate length in the lattice. In this case only loops with an even number of sites will be allowed and hence only even powers of $\mathcal{U}$ will survive the trace operation.

The second derivative of the effective action is given by:

$$\left(\frac{\partial^2 S_{eff}}{\partial z_i^2}\right)\Big|_{z=0} = 2\sum_{k=0}^{\infty}\chi_{2(k+1)}\sum_{q=0}^{k} Sp[(\mathcal{U})^{2q}P_i(\mathcal{U})^{2(k-q)}P_i] \tag{4.4}$$

For vanishing interaction, $J \rightarrow 0$, we have:

$$(\frac{\partial^2 S_{eff}}{\partial z_i^2})\mid_{z=0} = -\frac{1}{2} \tag{4.5}$$

and S_{eff} itself vanishes. That assures the correct limiting value of the Path Integral and of the partition function; i.e. 2^N.

The full expression for B_i is:

$$B_i[\mathcal{U}] = 1 + .2\sum_n Sp[\frac{1}{i\omega_n - c\mathcal{U}}P_i\frac{1}{i\omega_n - c\mathcal{U}}P_i] \tag{4.6}$$

The effects of the constraint are entirely contained in the functionals $B_i[\mathcal{U}]$. As we anticipated before the effect of the constraint is to reduce the entropy contribution to the total effective action. That is what one would aspect on physical grounds, resulting from the reduction of the available portion of the Hilbert space due to the enforcing of the half filling projector.

It is very important to prove that the average of the occupation number operator on the site i, is exactly equal to one. We can easily prove it for a square lattice and in the static approximation for the auxiliary fields $\mathcal{U}_{ij}$. Indeed we have:

$$< n_i >= Z^{-1}\left[\frac{\partial}{\partial z_i}\mathcal{P}\mathcal{Z}[z]\right]_{z=0} = Z^{-1}\int\prod_{(i,j)} d^2\mathcal{U}_{ij}\left[-\frac{\partial S_{eff}}{\partial z_i}+\sum_{k=1}^{N} B_k^{-1}\frac{\partial B_k}{\partial z_i}\right]_{z=0}\cdot$$
$$\exp\left(-\pi\sum_{(i,j)} \mid \mathcal{U}_{ij}\mid^2 - S_{eff} + \sum_k \ln(4B_k)\right) \qquad (4.7)$$

where:

$$\frac{\partial B_k}{\partial z_i} = \frac{\partial^3 S_{eff}}{\partial z_i \partial z_k^2} - 2\frac{\partial^2 S_{eff}}{\partial z_i \partial z_k}\left(1+\frac{\partial S_{eff}}{\partial z_k}\right) \qquad (4.8)$$

and, at z=0, $\partial S_{eff}/\partial z_i|_{z=0} = -1$. So that to prove $< n_i >= 1$ we have to prove that the third derivative of the effective action vanishes. In fact, we have:

$$\frac{\partial^3 S_{eff}}{\partial z_i^2 \partial z_k} = -4\sum_n Sp\{\chi_n^+ P_i \chi_n^+ P_i \chi_n^+ P_k\} \qquad (4.9)$$

where $\chi_n^+ = (i\omega_n - c\mathcal{U})^{-1}$ (see Appendix A for explicit derivations), and this third derivative is explicitely an odd function of $\tilde{\mathcal{U}}$. We now argue that this derivative is always zero when calculated at $z = 0$ In this case we have $\tilde{\mathcal{U}} = -c\mathcal{U}$. The expansion of the previous term gives:

$$\frac{\partial^3 S_{eff}}{\partial z_i^2 \partial z_k} = -4\sum_n\left(\frac{1}{i\omega_n}\right)\sum_{h,q,l}\left(\frac{1}{i\omega_n}\right)^{h+q+l} c^{h+q+l} Sp\{\mathcal{U}^h P_i \mathcal{U}^q P_i \mathcal{U}^l P_k\} \qquad (4.10)$$

Frequency sum forces $h+q+l$ to be odd. Moreover:

$$Sp\{\mathcal{U}^h P_i \mathcal{U}^q P_i \mathcal{U}^l P_k\} = (\mathcal{U}^h)_{ki}(\mathcal{U}^q)_{ii}(\mathcal{U}^l)_{ik} \qquad (4.11)$$

with no summations on i and k. On a square lattice, $(\mathcal{U}^q)_{ii}$ must contain an even number of $\mathcal{U}$'s so that q must be an even number. To go from site i to site k one can

make only an even or an odd number of steps whatever path in the lattice is chosen. So, h and l must be both even or odd. But then $h+q+l$ cannot be odd. This proves that the third derivative of the effective action is equal to zero and finally, that the average on-site occupation number is exactly equal to one.

The solution with $\mathcal{U}_{ij}$ constants is not a minimum due to the perfect nesting instability. It appears that the minimum amount of symmetry breaking which allow a locally stable minimum is an increase of the unit cell length by a factor $\sqrt{2}X\sqrt{2}$. Following AM, we restrict the random fields $\mathcal{U}_{ij}$ to be translationally invariant along the diagonals of the square lattice. The rapresentation of the fields $\mathcal{U}_{ij}$ and of the projectors P_i in Fourier space will considerably simplify the calculations.

The resulting bipartite lattice will be made of even sites surrounded by odd sites and viceversa. This correspond to a doubbling of the unit cell and leads to an halved Brillouin zone, i.e. a reduced Brillouin zone (RBZ).

Denote by the lattice site indices the basis of Wannier states: $\mid i >$. We want to perform a change from this basis to a basis denoted by: $\mid \alpha, k >$ where k is in the RBZ and α takes two values, even or odd, distinguishing the two sublattices. These new states are eigenfunctions of the translation operators along the diagonals, $\vec{a} = \hat{x} + \hat{y}$, $\vec{b} = \hat{x} - \hat{y}$:

$$T_{\vec{a},(\vec{b})} \mid \alpha, k >= e^{-i\vec{k}\vec{a},(\vec{b})} \mid \alpha, k > \tag{4.12}$$

As usual we have that the two basis are related by:

$$< i \mid \alpha, k >= \sqrt{\frac{2}{N}} e^{i\vec{k}\cdot\vec{R}_i} \delta_{i,\alpha} \tag{4.13}$$

Then for the matrix $\mathcal{U}_{ij}$ we have:

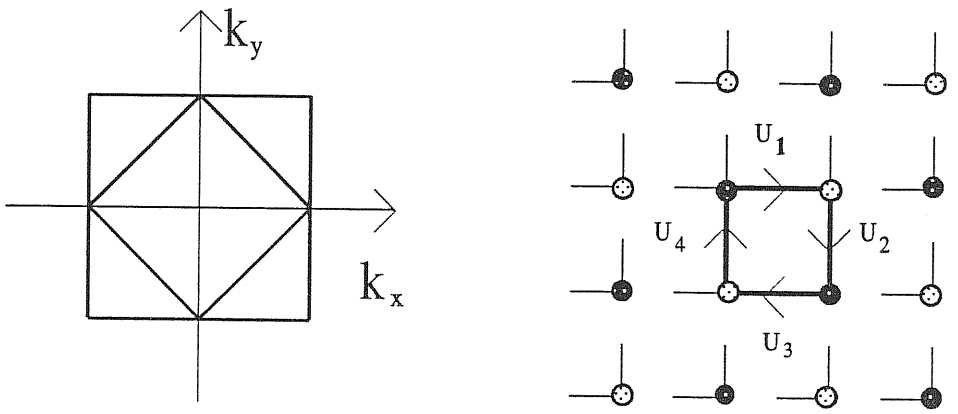

Figure 4.1: The Reduced Brillouin Zone and the bipartite lattice with definitions of the auxiliary fields

$$\begin{aligned} < \alpha, k \mid \mathcal{U} \mid \beta, h > &= \sum_{i,j} < \alpha, k \mid i > \mathcal{U}_{ij} < j \mid \beta, h > \\ &= \frac{2}{N} \sum_{i,j} e^{-i\vec{k}\cdot\vec{R}_i} \mathcal{U}_{ij} e^{i\vec{h}\cdot R_j} \delta_{i,\alpha} \delta_{j,\beta} \end{aligned} \tag{4.14}$$

It easy to see that $\mathcal{U}$ will be diagonal in the indices $\vec{k}$ and antidiagonal in the indices α. $\mathcal{U}_{ij}$ will connect only nearby sites lying in different sublattices and will be parametrized by four indipendent complex fields $\mathcal{U}_{1,2,3,4}$. We introduce the matrix elements of the auxiliary fields as:

$$< o, \vec{k} \mid \mathcal{U} \mid e, \vec{h} >= \delta_{\vec{k},\vec{h}} \lambda(\vec{k}) \tag{4.15}$$

where:

$$\lambda(\vec{k}) = \mathcal{U}_1 e^{ik_x} + \mathcal{U}_2^* e^{-ik_y} + \mathcal{U}_3 e^{-ik_x} + \mathcal{U}_4^* e^{ik_y} \tag{4.16}$$

The convention are depicted in the figure (4). The lattice constant is taken to be unity.

Similarly one can construct the matrix elements of the projector:

$$\begin{aligned} < \alpha, \vec{k} \mid P_i \mid \beta, \vec{h} > &= \sum_{l,m} < \alpha, \vec{k} \mid l >< l \mid P_i \mid m >< m \mid \beta, \vec{h} > \\ &= \frac{2}{N} e^{i(\vec{h}-\vec{k})R_i} \delta_{\alpha,\beta} \delta_{\alpha,i} \end{aligned} \tag{4.17}$$

that is diagonal in the α indices. Note that the matrix $\mathcal{U}$ can be easily diagonalized and its eigenvalues are $\pm E(\vec{k})$ and $E(\vec{k}) = \mid \lambda(\vec{k}) \mid$. $\mathcal{U}^2$ will be diagonal with doubly degenerate eigenvalues: $E^2(\vec{k})$.

The $\lambda(\vec{k})$'s have already been introduced by AM. However, due to the presence of the constraint, they cannot be interpreted anymore, in a straightforwrd way, as quasiparticle's energies at the mean field level as they did in their original work. We come back to this point later.

Given these approximations we can evaluate $S_{eff}[c\mathcal{U}]$ in terms of the eigenvalues of the matrix $\mathcal{U}^2$.

$$S_{eff}[\mathcal{U}] = 2 \sum_{h=1}^{\infty} \frac{(-1)^{2h}}{2h} \chi_{2h} Sp[(\mathcal{U}^2)^h c^{2h}] = \sum_{h=1}^{\infty} \frac{\chi_{2h}}{h} Sp[(\mathcal{U}^2)^h c^{2h}] \tag{4.18}$$

where $\chi_{2h} = \sum_n (i\omega_n)^{-2h}$.

Introducing a dimensionless coupling constant g, $g \in (0, c)$, by letting $c\mathcal{U} \to g\mathcal{U}$ and differentiating with respect to g, after a standard summation on the Matsubara frequencies, we find:

$$\frac{\partial}{\partial g} S_{eff}[g\mathcal{U}] = -2 \sum_k E(k) \tanh\left(\frac{gE(k)}{2}\right) \tag{4.19}$$

This last equation can be easily integrated, yielding:

$$S_{eff}[\mathcal{U}] = -4 \sum_k \ln\cosh\left(\frac{cE(k)}{2}\right) \tag{4.20}$$

After some straightforward algebra the constraint contribution becomes:

$$\begin{aligned} B_i = 1 \quad - \quad & \frac{1}{c}\left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{1}{E(k)^2 - E(k')^2} \cdot \\ & \left(E(k)\tanh(\frac{cE(k)}{2}) - E(k')\tanh(\frac{cE(k')}{2})\right) \end{aligned} \tag{4.21}$$

indipendently of the site index i.

The first term in the total effective action is:

$$\pi \sum_{(i,j)} \mid \mathcal{U}_{ij} \mid^2 = \pi \frac{N}{2} \sum_{i=1}^{4} \mid \mathcal{U}_i \mid^2 \tag{4.22}$$

This term suggests that values of the order parameters $\mathcal{U}_i$ of physical significance should scale with $\sqrt{\beta}$. We define new dimensionless order parameters as:

$$\begin{aligned} d_i &= \frac{c}{\beta J}\mathcal{U}_i \\ d_k &= \frac{c}{\beta J}\lambda(k) \\ x_k &= cE(k) \end{aligned} \tag{4.23}$$

The total effective action now reads:

$$\beta\mathcal{F}_{eff} = N\beta J \sum_i \mid d_i \mid^2 -4 \sum_k \ln\cosh(x_k/2) - N \ln 4B \tag{4.24}$$

and

$$B = 1 - \left(\frac{2}{N}\right) \sum_{k,k'} \frac{x_k \tanh(x_k/2) - x_{k'} \tanh(x_{k'}/2)}{x_k^2 - x_{k'}^2} \tag{4.25}$$

Again, when $J \to 0$, $B \to 1/2$ for any temperature. On the other hand, at zero temperature, we have $B = 1$ no matter what d is. Therefore B decreases smoothly from 1 to $1/2$ when the temperature increases. This means that, for any configuration, the effect of the constraint is to reduce the entropy term in the total effective action.

4.1 Mean field phases

Minimization of the effective total action yelds the mean field configurations of the order parameters d_k.

The self consistency procedure runs as follows:

$$\frac{\partial\beta\mathcal{F}}{\partial\mathcal{U}^\star} = \pi\frac{N}{2}\mathcal{U} - 2\sum_k \frac{\partial x_k}{\partial\mathcal{U}^\star} \cdot \mathcal{D}_k = 0 \tag{4.26}$$

where

$$\mathcal{D}_k = \tanh(x_k/2) - \frac{4}{NB}\sum_{k'} D(x_k, x_{k'}) \tag{4.27}$$

and the second term introduced by the constraint is:

$$D(x,y) = \frac{1}{(x^2-y^2)^2}\left(\frac{x(x^2-y^2)}{2\cosh(x/2)} - (x^2+y^2)\tanh(x/2) + 2xy\tanh(y/2)\right) \tag{4.28}$$

From equation (4.26) one can build up a self consistency equation for the order parameters d_q defined via equations (4.23), (4.16):

$$d_q = \frac{2}{N}\sum_k(\cos(q_x - k_x) + \cos(q_y - k_y))\mathcal{D}_k\frac{d_k}{x_k}t \tag{4.29}$$

We are in position now to generalize the work by AM to include the constraint within the saddle point approximation. We collect here the results for the dimers or Peierls phase and for the Flux phase which are still found as extrema of our effective action. The dimer phase considered here is altermating on the bonds, so that the translational symmetry along the diagonals of the lattice is preserved according to the ansatz of eq.(4.16).

a) Peierls phase

This phase is, in mean field approximation, a bond-centered charge density wave in which each site forms a dimer with one of its nearest nieghbours and in fact break the translational symmetry. Here the electrons are localized on individual dimers and the electronic excitation spectrum turns out to be completely gapped.

In our case the interpretation in term of quasiparticle spectrum is no longer true but the characteristic of the phase are always the same.

Here only one of the d_i's fields is different form zero and it may be made real by a gauge transformation.

$$d_1 = d \qquad\qquad d_2 = d_3 = d_4 = 0 \tag{4.30}$$

We have for the constraint term :

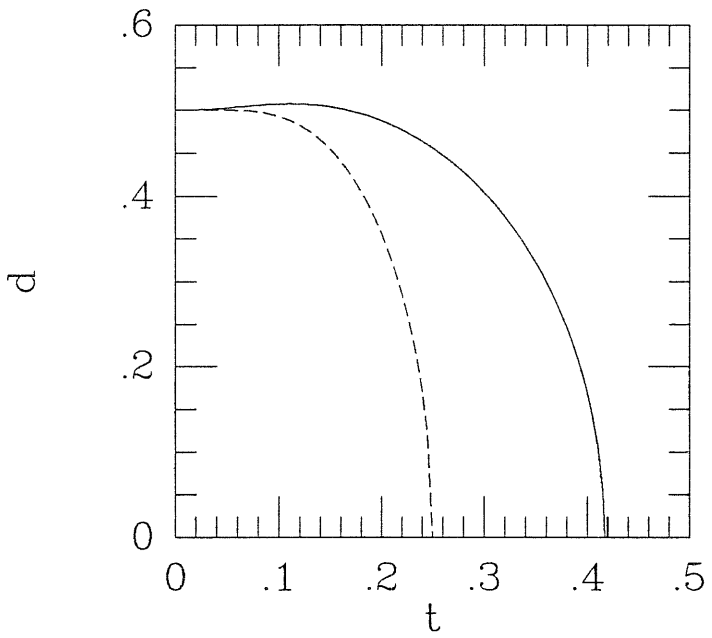

Figure 4.2: Temperature dependence of the order parameter d as a function of the reduced temperature in the presence (full curve) and in the absence (dashed curve) of the constraint.

$$B_P = 1 - \frac{1}{4}\left(\frac{\tanh x}{x} + \frac{1}{\cosh^2 x}\right) \tag{4.31}$$

and we define:

$$D_P = \frac{\partial}{\partial x} \ln B_P \mid_{x=d/2t} \tag{4.32}$$

The self consistency equation for the order parameter is:

$$2d = \tanh \frac{d}{2t} + \frac{1}{2} D_P \tag{4.33}$$

In figure (4.2) is drawn the temperature dependence of the order parameter d as a function of the reduced temperature $t = \frac{1}{\beta J}$ in presence (full curve) and in absence (dashed curve) of the constraint.

The mean field transition temperature is found to be higher ($t_c = 5/12$), than that found in the absence of the constraint ($t_{co} = 1/4$).

b) Flux phase

In order to leave the Lagrangian invariant under the local U(1) gauge transformation, the auxiliary fields $\mathcal{U}_{ij}$ must transform as link variables of a lattice Abelian gauge theory. We can identify the phase of $\mathcal{U}_{ij} =\mid \mathcal{U} \mid e^{i\phi_{ij}}$ as a spatial gauge field A through $\phi_{ij} = \int_i^j \vec{A} \cdot d\vec{l}$. Going to the four link variables d_i the plaquette operator:

$$\prod_i d_i = d_1 d_2 d_3 d_4 =\mid d_1 \mid\mid d_2 \mid\mid d_3 \mid\mid d_4 \mid e^{i\Phi} \tag{4.34}$$

has to be gauge invariant. By Stoke's theorem, Φ is the flux due to a fictitious magnetic field penetrating the plaquette.

$$\Phi = \sum_{\square} \phi_{ij} = \oint \vec{A} \cdot d\vec{l} \tag{4.35}$$

The Flux phase here considered carries 1/2 quantum flux per plaquette, (per hole in our half filling case). A special choise of the gauge which makes the phases equal among the bonds is:

$$d_i = de^{i\pi/4} \qquad \forall i \tag{4.36}$$

and $d(k) = 2d(\cos(k_x) - i\cos(k_y))$.

We recall that the translational invariance, along the diagonals of the original square lattice, implies that the k vectors span the RBZ. In the thermodynamic limit, the momentum sums can be converted into integrals according to:

$$\frac{2}{N}\sum_k \ldots \rightarrow \int_{RBZ} \frac{d^2k}{2\pi^2}\ldots \tag{4.37}$$

We define $\epsilon_k = (\cos k_x^2 + \cos k_y^2)^{1/2}$ and $\bar{\epsilon} = \int \frac{d^2k}{2\pi^2}\epsilon_k = 0.918$.

In this case the self consistency equation for the order parameter reads:

$$4d = \int_{RBZ} \frac{d^2k}{2\pi^2}\epsilon_k \tanh\frac{d\epsilon_k}{t} + \frac{t}{2B}\delta B \tag{4.38}$$

where:

$$\delta B = \int_{RBZ} \frac{d^2k}{2\pi^2}\left(\frac{t}{d^2}\int_{RBZ}\frac{d^2k'}{2\pi^2}\frac{\epsilon_k}{\epsilon_k^2-\epsilon_{k'}^2}\tanh\frac{\epsilon_k d}{t} + \right.$$
$$\left. + \frac{1}{d}\int_{RBZ}\frac{d^2k'}{2\pi^2}\frac{\epsilon_k^2}{\epsilon_k^2-\epsilon_{k'}^2}\tanh^2\frac{\epsilon_k d}{t} - \frac{1}{2d}\right) \tag{4.39}$$

The transition temperature is found to be equal to that of the Peierls phase, both in presence and in absence of the constraint. The behaviour of the order parameter as a function of the reduced temperature is plotted in Figure (4.3).

4.2 Free Energy

Within mean field approximation the free energy is just given by the effective total action of eq.(4.24):

$$\beta\mathcal{F}_{eff} = N\beta J\sum_i \mid d_i \mid^2 -4\sum_k \ln\cosh(x_k/2) - N\ln 4B \tag{4.40}$$

evaluated at the configurations of stationarity we have described in the previous chapter.

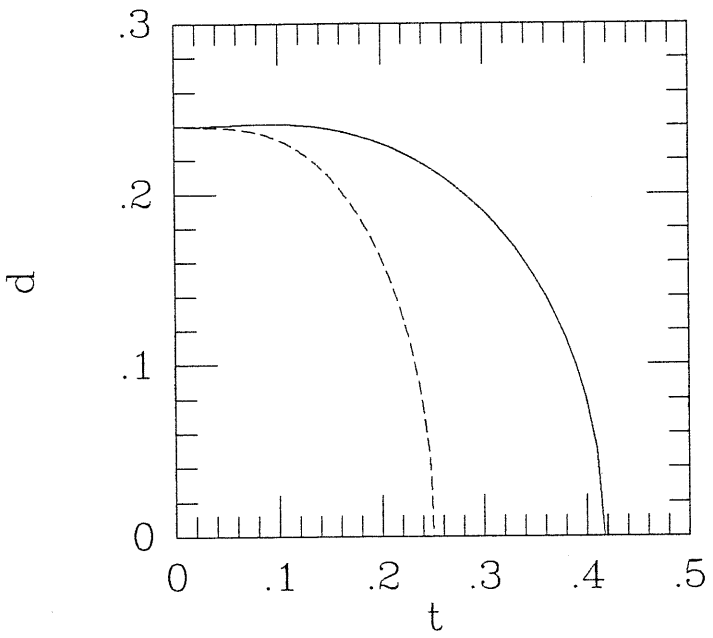

Figure 4.3: The order parameter in the Flux phase as a function of the reduced temperature inpresence (full curve) and in absence (dashed curve) of the constraint.

In absence of the constraint the expression for $\mathcal{F}$ can be easily interpreted as what results from non interacting fermions with single particles energies given by $\pm E(k)$.

This is an essentially classical result in the theory of path integrals [42]. A saddle point evaluation of a path integral yields the value of the free energy one would obtain by performing a mean field (Hartree) approximation on the original Hamiltonian. There is no reason however for the theorem to hold true also in the case of constrained path integrals as those we are considering here. For this reason we will call "generalized mean field approximations" those corresponding to an evaluation of the free energy at its stationary points. It may not be possible to identify a quasiparticle spectrum in a straightforward way, as in the usual mean field approximation. In particular the $E(k)$'s introduced before are useful parameters which however do not define quasiparticle excitation spectrum, unless one sets $B = 1$. In the general case we expect the quasiparticle energy spectrum, identified

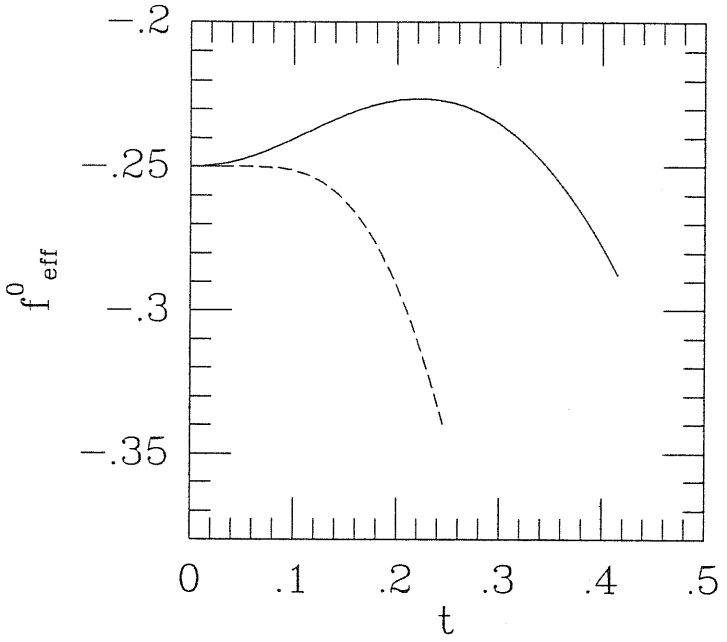

Figure 4.4: Free energy per particle versus temperature in presence (full curve) and in absence (dashed curve) of the constraint (Peierls phase)

through the poles of appropriate Green's functions, to be given by functions of $E(k)$ that reduce to the latter when $B = 1$.

We find that in presence of the constraint, the effective total action of eq.(4.24) cannot even be considered as the mean field approximation to a physically meaningful free energy. In fact it shows the wrong temperature dependence for both phases.

The effective free energy for the Peierls phase is given by:

$$f^0_{eff} = \frac{\mathcal{F}^0_{eff}}{NJ} = d^2 - 2t\ln(\cosh(d/2t)) - t\ln 4B_P(d/2t) \tag{4.41}$$

The zero temperature results are the same as the AM results, i.e. $d(t=0) = 1/2$ and $f^0_{eff}(t=0) = -1/4$.

In figure (4.4) is plotted the free energy per particle versus temperature in presence (full curve) and in absence (dashed curve) of the constraint.

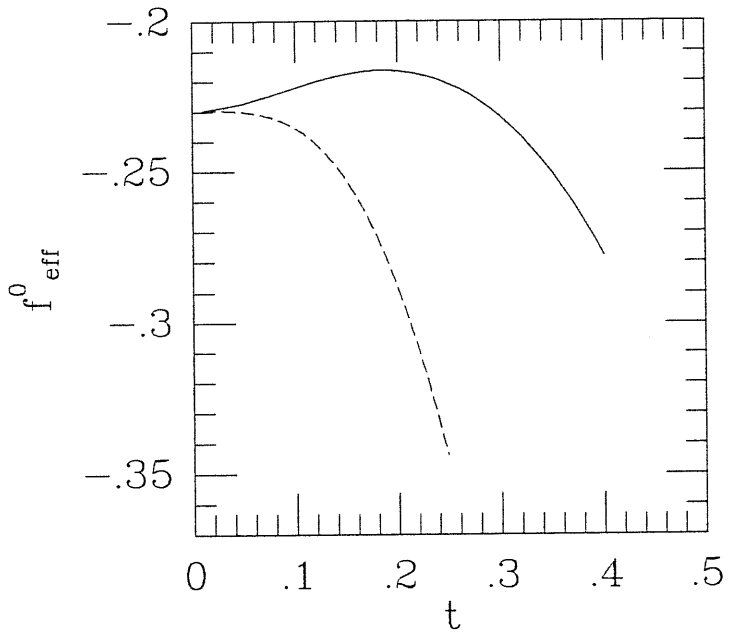

Figure 4.5: Free energy per particle versus temperature in presence (full curve) and in absence (dashed curve) of the constraint (Flux phase)

As the same as before we have for the Flux phase that the effective free energy is given by:

$$f^0_{eff} = 4d^2 - 2d\bar{\epsilon} - 2t\int_{RBZ}\frac{d^2k}{2\pi^2}\ln(1+e^{2d\epsilon_k/t}) - t\ln B \qquad (4.42)$$

One finds, for t=0, the results of AM: $\mathrm{d}(t=0) = \bar{\epsilon}/4$ and $f^0_{eff}(t=0) = -\bar{\epsilon}^2/4 = -0.2295$.

But the temperature dependence of the saddle point free energy plotted in Fig.(4.4) for the Peierls phase and in Fig.(4.5) for the Flux phase turn out to be unphysical when the constraint is included.

Due to the limited contribution coming from the entropy of the saddle point configurations, appearing in the free energies, the latter are found to increase with the temperature in a certain range of temperature. Such a behaviour would yield a negative entropy at those temperatures. This implies that the bare saddle point contribution to the free energy

is not enough and gaussian fluctuations should also be included, at least.

5 Gaussian fluctuations

In this chapter we calculate the gaussian fluctuations of the total effective action due to variations of the the auxiliary fields $\mathcal{U}_i$'s around their stationary values. We consider only fluctuations of the same space periodicity as our saddle point solutions. They are also chosen to be static so that quantum fluctuations are excluded;

$$\delta\lambda(k) = \delta\mathcal{U}_1 e^{ik_x} + \delta\mathcal{U}_2^\star e^{-ik_y} + \delta\mathcal{U}_3 e^{-ik_x} + \delta\mathcal{U}_4^\star e^{ik_y} \tag{5.1}$$

and $\delta\lambda^\star(k)$ which is considered as indipendent; i.e. we vary separately both the real and imaginary parts of the four plaquette fields $\delta\mathcal{U}_i$.

This provides a qualitative measure of the stability of the saddle point solutions, with respect to this type of fluctuations. We do not reproduce the result by Dombre et al.[24] which shows instability of the flux phase with respect to a "box" phase which is defined in a $2X2$ unitary cell. Similarly the instability of our alternating Peierls phase with respect to the columnar one with a $2X1$ unitary cell is also ruled out [23].

The global symmetries of the action are also found as zero eigenvalues of the $8X8$ curvature matrix. These zero modes correspond to the residual gauge symmetries which are not broken by the mean field solutions.

Non zero modes give the collective excitations that are examined for the two studied phases.

We can also evaluate the mean square fluctuations of the order parameter corresponding to the eigenvalues which give the most divergent fluctuations as a function of temperature and compare it in presence and in absence of the constraint.

These mean square fluctuations give the temperatures, according to the Ginzburg Landau criterion, at which there is the breakdown for mean field solutions and the onset of criticality.

These calculations allow us not only to point out the amuont at which thermal fluctuations around the mean field solutions are depressed as an effect of the half filling constraint but also to recover a correct behaviour for the effective free energy versus temperature when the contribution of these fluctuations to the free energy is added.

Our starting point if the effective free energy:

$$\beta\mathcal{F}[\mathcal{U}] = N\pi \sum_{i=1}^{4} \mid \mathcal{U} \mid^2 + S_{eff}[\mathcal{U}] - N \ln 4B[\mathcal{U}] \tag{5.2}$$

where, recalling that we defined $x_k = cE(k)$:

$$S_{eff}[\mathcal{U}] = -4 \sum_{k} \ln \cosh \frac{x_k}{2} \tag{5.3}$$

and

$$B = 1 - \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{x_k \tanh x_k/2 - x'_k \tanh x'_k/2}{x_k^2 - x_k'} \tag{5.4}$$

Here we give only the final results obtained after the trace is performed in Fourier space and the Matsubara frequency summations are performed using standard contour

integral techniques. The Appendix A contains the general line of calculations.

The complete expression for the second variation of the total effective action per particle, in units of J, is:

$$\delta^2 f_{eff} = 2\sum_{i=1}^{4} \mid \delta d_i \mid^2 + \frac{t}{N}\delta^2 S_{eff} - t\left(\frac{\delta^2 B}{B} - \frac{(\delta B)^2}{B^2}\right) \tag{5.5}$$

Explicit calculations can be found in Appendix A. Here:

$$\sum_{i=1}^{4} \mid \delta d_i \mid^2 = \left(\frac{2}{N}\right)\sum_{k} \mid \delta d_k \mid^2 \tag{5.6}$$

$$\frac{t}{N}\delta^2 S_{eff} = 2\left(\frac{2}{N}\right)\sum_{k}\left(Q(\mid d_k \mid) \mid \delta d_k \mid^2 + \Re\left[\delta d_k \left(\frac{d_k}{\mid \delta d_k \mid}\right)^2 q(\mid d_k \mid)\delta d_k\right]\right) \tag{5.7}$$

where:

$$Q(\mid d_k \mid) = -\frac{1}{\mid d_k \mid}\tanh\frac{\mid d_k \mid}{2t} - \frac{1}{8t\cosh^2(\frac{\mid d_k \mid}{2t})} \tag{5.8}$$

and

$$q(\mid d_k \mid) = \frac{1}{\mid d_k \mid}\tanh\frac{\mid d_k \mid}{2t} - \frac{1}{8t\cosh^2(\frac{\mid d_k \mid}{2t})} \tag{5.9}$$

In absence of the constraint the gap equation is readly written in terms of Q and q as:

$$1 + Q - q = 0 \tag{5.10}$$

The contributions due to the constraint given by δB and $\delta^2 B$ are reported in Appendix A.

The variations of the complex variables d_i's and d_i^*'s around their equilibrium values, change the free energy according to an 8X8 curvature matrix.

If we exclude zero modes we will find a positive determinant so that the two saddle point solutions studied are infact local minima and are stable with respect to this type of fluctuations. The curvature itself provides a qualitative measure of the stability.

5.1 Zero modes

Because of the chosen symmetry for the random auxiliary fields d_i, we end up with an order parameter with four complex components. Therefore, the dynamical matrix around the stationary point solutions is an 8X8 matrix. Its diagonalization gives us eight normal modes. Four out of these are amplitude modes:

$$d_l \rightarrow (1 + \delta\theta_l) \mid d \mid e^{i\pi/4} \tag{5.11}$$

therefore,

$$\frac{\delta d_l}{d} = \delta\theta_l \tag{5.12}$$

is a real quantity. The other four modes are phase modes:

$$d_l \rightarrow (1 + i\delta\theta_l) \mid d \mid e^{i\pi/4} \tag{5.13}$$

and therefore,

$$\frac{\delta d_l}{d} = i\delta\theta_l \tag{5.14}$$

turns out to be a pure imaginary quantity. Among the phase modes there can be Goldstone modes corresponding to global symmetries of the total effective action that are not broken by the mean field solutions. The corresponding eigenvectors give the phase space directions for the fluctuating fields that leave the total effective action unchanged. They have zero eigenvalues.

Consider an element g of the invariance group of $\mathcal{F}_{eff}$ which is parametrized by a continous variable θ, $g = g(\theta)$. The application of g to the mean field solution is still a solution of the mean field equation, $gd_i^{m.f.} = d_i^{m.f.}(\theta)$. Because $g\mathcal{F}$ does not depend on θ,

$$\frac{\delta \mathcal{F}}{\delta \theta} = \frac{\delta \mathcal{F}}{\delta d}\frac{\partial d}{\partial \theta} = 0 \tag{5.15}$$

Therefore, $\frac{\partial d_i^{m.f.}(\theta_0)}{\partial \theta_0}$ is an eigensolution of the first variation of the total effective action.

The number of these independent Goldstone modes is the order of the reamining symmetry group of the system in the ordered phase. The first of these mode is immediately recognizable: it is the U(1) symmetry mode

$$d_k \rightarrow d_k e^{i\theta} \tag{5.16}$$

It is easy to show that the gauge transformation $U(1)$ leaves the free energy unchanged both for the Pierels and the Flux phase. We can calculate, in absence of constraint, the second variation contribution to the free energy due to $\delta d_k = id\delta\theta$:

$$\delta^2 S = \frac{2}{N}\sum_k \mid d_k \mid^2 (1 + Q(\mid d_k \mid) - \Re\{q(\mid d_k \mid)\})(\delta\theta)^2 \tag{5.17}$$

In the Peierls phase $\mid d_k \mid = d$ and we have:

$$\delta^2 S = \left(1 - \frac{1}{2d}\tanh\frac{d}{2t}\right)(\delta\theta)^2 = 0 \tag{5.18}$$

due to the gap equation (4.33).

In the Flux phase $\mid d_k \mid = 2d\epsilon_k$ and

$$\delta^2 S = \frac{2}{N}\sum_k \left(4d^2\epsilon_k^2 - d\epsilon_k \tanh\frac{d\epsilon_k}{t}\right)(\delta\theta)^2 = 4d^2 - d4d = 0 \tag{5.19}$$

using again the gap equation (4.38).

This is the only zero mode in the Peierls phase. For the flux phase two other zero modes are found:

The second zero mode corresponds to:

$$\begin{aligned} d_1 &\rightarrow d\, e^{-i\theta_2} \\ d_3 &\rightarrow d\, e^{i\theta_2} \\ d_{2,4} &\rightarrow d \end{aligned} \tag{5.20}$$

that gives:

$$\frac{\partial \mathbf{d}}{\partial\theta_2} = i\, d \begin{pmatrix} -e^{-i\theta_2} \\ 0 \\ e^{i\theta_2} \\ 0 \end{pmatrix} \tag{5.21}$$

Where $\mid d_k \mid \rightarrow 2\, d\tilde{\epsilon}_k$, with $\tilde{\epsilon}_k = \mid \cos(k_x - \theta_2) - i\cos(k_y) \mid$.

The third transformation is given by:

$$\begin{aligned} d_{1,3} &\rightarrow d \\ d_2 &\rightarrow d\, e^{-i\theta_3} \\ d_4 &\rightarrow d\, e^{i\theta_3} \end{aligned} \tag{5.22}$$

that gives:

$$\frac{\partial \mathbf{d}}{\partial \theta_3} = i\, d \begin{pmatrix} 0 \\ -e^{-i\theta_3} \\ 0 \\ e^{i\theta_3} \end{pmatrix} \tag{5.23}$$

Here $d_k \rightarrow 2\ de^{i\pi/4}(\cos(k_x) - i\ \cos(k_y - \theta_3))$.

In Appendix B the proofs that these modes do not change the total effective action are given.

5.2 Collective excitations

Diagonalization of the dynamical matrix of the fluctuations around the stationary point solutions (whose explicit calculations are reported in Appendix C) leads to the following results:

a) Peierls phase

A part from the zero mode described previously, there is one non degenerate mode with eigenvalue λ_2 and six degenerate modes with eigenvalue λ_1.

We have noticed that the zero mode is associated with a phase change of d_1. We can easily see that the λ_2 mode, wich is an amplitude mode, is associated with a change in the

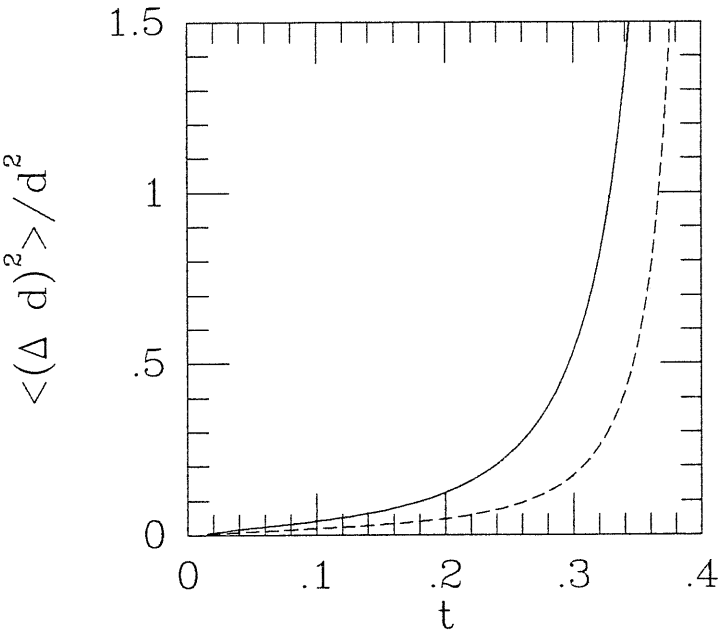

Figure 5.1: Mean square fluctuations of the order parameter in the Peierls phase as a function of the reduced temperature. (Full curve corresponds to λ_2, dashed curve corresponds to λ_1.

amplitude of d_1. It is physically reasonable to see that it takes the largest value because our free energy directly depend on $\mid d_1 \mid$. The remaining six eigenmodes will be associated to changes in amplitudes and phases of d_2, d_3, d_4.

The corresponding mean square fluctuations of the order parameter:

$$\frac{<(\Delta d)^2>}{d^2} = \frac{t}{4\lambda_i d^2} \tag{5.24}$$

plotted in Figure (5.2) as a function of the reduced temperature t, are lower for the first mode than for the second degenerate modes.

b) Flux phase

Here we have found three zero modes which are phase modes related to the possibility of changing arbitrarily three phases of the order parameter keeping the total phase in the

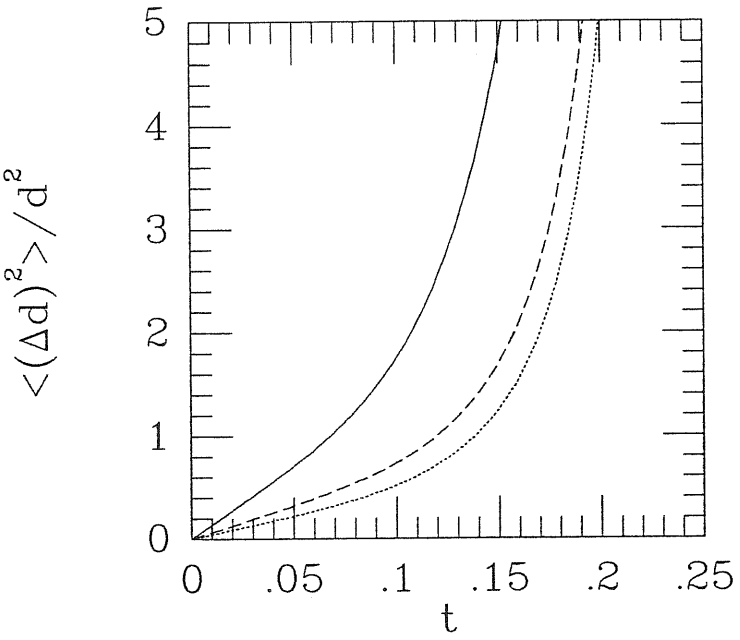

Figure 5.2: Mean square fluctuations of the order parameter in the Flux phase as a function of the reduced temperature. (Full curve corresponds to λ_1, dashed curve corresponds to λ_2 and dotted curve corresponds to λ_3.

elementary plaquette fixed to be equal to π. Therefore, the collective excitations are given by one phase mode which changes the total flux in the plaquette (dashed line in Fig.5.2), one amplitude mode (dotted line in Fig. 5.2) which changes the modulus of the order parameter and three degenerate amplitude modes (full line in Fig.5.2) which change the relative amplitude of d_1, d_2, d_3, d_4 keeping $\mid d_k \mid$ fixed.

The corresponding mean square fluctuations, plotted in figure (5.2) as a function of the reduced temperature, are higher for the three degenerate amplitude mode, λ_1. That is what one would expect on physical ground because our free energy depend explicitely only on the modulus of d_k and on the total flux in the plaquette.

5.3 Single particle excitation spectrum

We do not consider the constraint at the moment and assume that the single particle excitation spectrum can be deduced from the energies $\pm E_k = \pm c \mid \lambda(k) \mid$. We note that, in the Flux phase these cannot be considered as single particle energies because they are gauge dependent. In fact in the case of the three zero modes they change with the symmetry parameters θ_1, θ_2 and θ_3 as:

$$\begin{aligned} E_k^1 &= \mid \cos k_x - i \cos k_y \mid \\ E_k^2 &= \mid \cos(k_x - \theta_2) - i \cos k_y \mid \\ E_k^2 &= \mid \cos k_x - i \cos(k_y - \theta_3) \mid \end{aligned} \tag{5.25}$$

This gauge dependence does not lead to any inconsistencies since the physical excitations consist of particle-hole pairs confined together on the same site.

As we mentioned before, in presence of the constraint, it is no more clear how to isolate quasiparticle energies from the free energy. In this case one should evaluate the single particle Green functions and identify single particle energies from their poles. In order to do that one should include from the beginning, in the generating *functional*, source fields coupled to the single particle creation and annihilation operators. The generating *function* we are dealing with at the moment should be replaced a generating functional as we outline shortly in the last chapter.

In the Flux phase we can construct a gauge invariant quantity out of the $\pm E_k$'s that is the single particle (particle-hole) excitation spectrum given by:

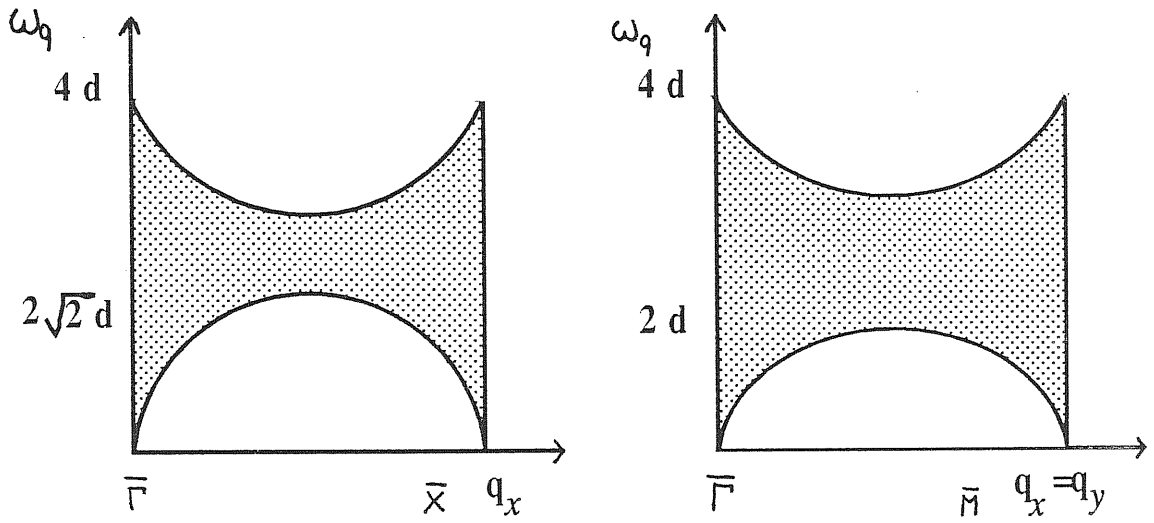

Figure 5.3: Schematic picture of the particle-hole excitation spectrum in the crystal directions Γ-M and Γ-X

$$\omega_q = \{E_{k+q} + E_k; k, k+q \in RBZ\} \tag{5.26}$$

where:

$$E_{k+q} + E_k = 2\ d\ \sqrt{\cos^2(k_x + q_x) + \cos^2(k_y + q_y)}\sqrt{\cos^2 k_x + \cos^2 k_y} \tag{5.27}$$

As one can see from the Fig.(5.3), the excitation spectrum has zero energy modes at $q = (0,0)$, $(0,\pi)$, $(\pi,0)$ and $q = (\pi,\pi)$. Therefore, the Lieb, Schultz and Mattis theorem saying that for half integer spin antiferromagnets there must either be broken translational symmetry or gapless excitations is satisfied by the flux phase solution. The translational symmetry is only apparently broken by our choise of the mean field solution in fact it can be easily recovered performing a gauge transformation.

In the Peierls phase the excitation spectrum, $\omega_q = 2\ d$, is completely gapped. In this

phase the translational symmetry is broken what again agrees with the LSM theorem.

6 Free Energy including Gaussian Fluctuations

While the Path Intergal for $\mathcal{Z}$ is unaffordable, the fields configurations which minimize the effective free energy are easily found.

The main result up to now is the writing of the partition function of the interacting system in the form:

$$\mathcal{Z} = \int \mathcal{D}\mathcal{U}_i \exp\left(-\beta \mathcal{F}_{eff}[\mathcal{U}_i]\right) \tag{6.1}$$

with $\mathcal{F}_{eff}$ given by equation (4.24). We have been able to integrate out the fermions at the cost of introducing a random external field seen by otherwise non interacting particles. Again we stress that only static fields will be considered. The lowest approximation to the evaluation of the path integral is the saddle point. This implies that a self consistent field is chosen which minimazes the effective free energy:

$$\frac{\delta \mathcal{F}}{\delta \mathcal{U}_i^*} = 0 \qquad\qquad i = 1, 2, 3, 4 \tag{6.2}$$

Within mean field approximation the free energy is just given by the evaluation of eq.(4.24) at the configurations of stationarity. As we noticed before, due to the limited contribution coming from the entropy this mean field value of the total effective action

was found to increase with the temperature in certain range of temperature. This is an unphysical behaviour and implies, of course, that the bare saddle point contribution to the free energy is not enough and gaussian fluctuation have to be included, at least. In order to do that, the path integral we want to perform is:

$$e^{-\beta \mathcal{F}_{eff}} = e^{-\beta \mathcal{F}^0_{eff}} \prod_{ij} \int d^2\delta d_{ij} e^{-\pi \delta d^* M' \delta d} \tag{6.3}$$

where, using the chosen symmetries for the 2N bonds variables, we have:

$$\prod_{ij} \int d^2\delta d_{ij} e^{-\pi \delta d^* M' \delta d} = \left[\prod_{i=1}^{4} \int d^2\delta d_i e^{-\pi \delta d^* M' \delta d} \right]^{\frac{N}{2}} \tag{6.4}$$

In the general case we can define the projection of the curvature matrix M' on the subspace orthogonal to the zero modes: $M'_\perp$. In block matrix form we have:

$$M' = \begin{bmatrix} 0 & 0 \\ 0 & M'_\perp \end{bmatrix} \tag{6.5}$$

The standard integration procedure[41], when the zero modes $\frac{\partial \mathbf{d}}{\theta_i}$ have been identified, gives:

$$\begin{aligned} \mathcal{Z} &= e^{-\beta \mathcal{F}^0_{eff}} \frac{1}{\sqrt{det M'_\perp}} \int \prod_{i=1}^{n} \frac{d\theta_i}{\sqrt{2\pi}} (det \mathcal{N})^{1/2} \\ &= \frac{1}{\sqrt{\prod'_i \lambda_i}} (2\pi)^{\nu/2} \gamma_\nu \end{aligned} \tag{6.6}$$

where the symbol 'prime' in the productory means the product of the non zero eigenvalues, ν is the number of zero modes and the $\nu X \nu$ matrix $\mathcal{N}$ has elements given by:

$$\mathcal{N}_{ij} = \sum_{l=1}^{4} \frac{\partial \mathcal{U}_l^*}{\partial \theta_i} \cdot \frac{\partial \mathcal{U}_l}{\partial \theta_j} \tag{6.7}$$

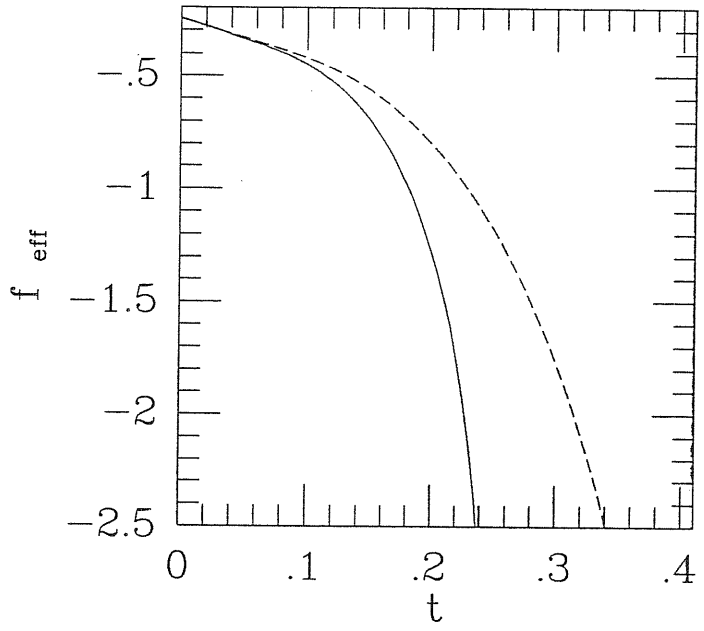

Figure 6.1: Reduced free energy per particle vs. reduced temperature (including gaussian fluctuations around the saddle point) for the Peierls phase without (broken line) and with the constraint (full curve).

Explicit calculations that can be found in Appendix D, give us:

$$\begin{aligned} &\nu = 1, && \gamma_1 = d && \text{in the Peierls phase} \\ &\nu = 3, && \gamma_3 = (2d^2)^{3/2} 1.203 && \text{in the Flux phase} \end{aligned} \tag{6.8}$$

a) Peierls phase

At the end of the day, for the Peierls phase, we get:

$$f_{eff} = f^0_{eff} - \frac{t}{2} \ln \left(\sqrt{\frac{1}{\lambda_1^6 \lambda_2}} d \right) \tag{6.9}$$

The result is plotted in Fig.(6.1) in presence and in absence of the constraint for comparison.

The effect of the constraint on this gaussian fluctuations is clearly seen in the plot

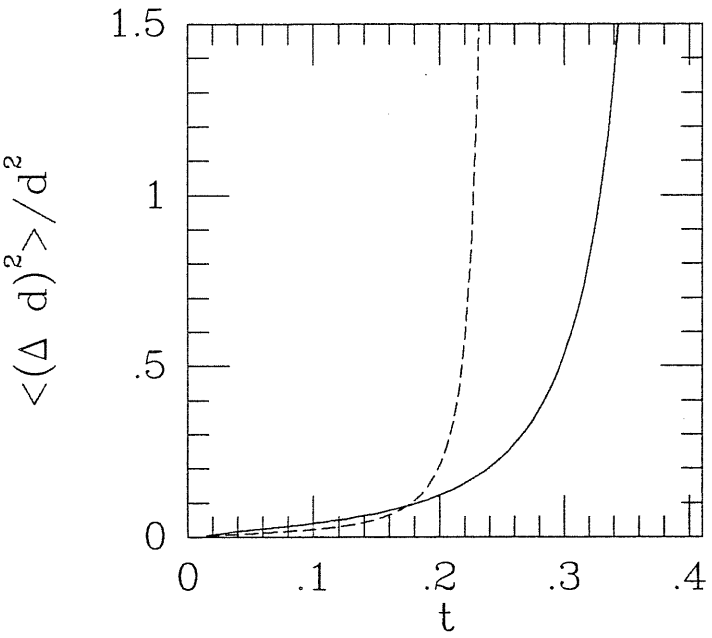

Figure 6.2: The relative mean square fluctuation of the order parameter vs. reduced temperature. Broken curve: Peierls phase without the single occupancy constraint. Full curve: Peierls phase including the constraint.

Fig.(6.2) of the mean square fluctuations of the order parameter, corresponding to the eigenvalue which gives the most divergent fluctuation, as a function of the temperature; i.e. $\frac{<(\Delta d)^2>}{d^2} = \frac{t}{4\lambda_1 d^2}$. One can easily see that the thermal fluctuations are depressed in presence of the constraint. In fact the temperature at which $\frac{<(\Delta d)^2>}{d^2}$ becomes of the order one increase from $t^\star = 0.22$ to $t^\star = 0.33$. This gives the signal of the breakdown of the mean field approximation and the onset of critical behaviour, according to the Ginzburg Landau criterion.

b) Flux phase

For the flux phase the final result for the free energy, plotted in Fig.(6.3) in presence and absence of constraint for comparison, is:

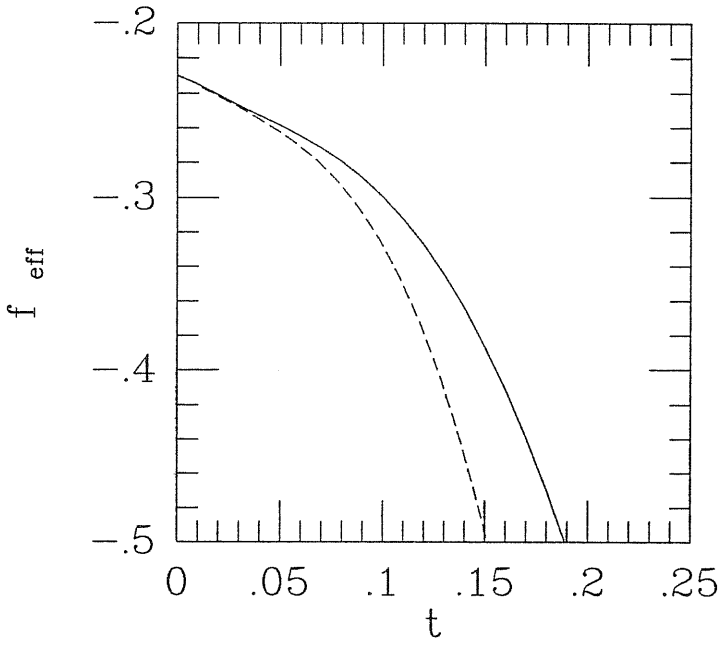

Figure 6.3: Effective free energy vs. reduced temperature including gaussian fluctuations for the flux phase. Broken curve: in absence of constraint. Full curve: in presence of constraint

$$f_{eff} = f^0_{eff} - \frac{t}{2}\ln\left(\gamma_3\sqrt{\frac{1}{\lambda_1^3\lambda_2\lambda_3}}\right) \tag{6.10}$$

Where $\gamma_3 = 1.2033(2d^2)^{3/2}$ comes from the integration of the zero modes over the angular variables θ_i's. (The explicit calculation can be found in the Appendix D).

The effect of the constraint on this gaussian fluctuations is clearly seen in the plot (Fig.(6.4)) of the mean square fluctuations of the order parameter, corresponding to the eigenvalue which gives the most divergent fluctuations, as a function of the temperature; i.e. $\frac{<(\Delta d)^2>}{d^2} = \frac{t}{4\lambda_2 d^2}$.

Also in the flux phase the thermal fluctuations are depressed in presence of the constraint even if the depression is less significative. In fact the signal of the breakdown of the mean field approximation and the onset of critical behaviour, according to the Ginzburg Landau criterion, given by the temperature at which $\frac{<(\Delta d)^2>}{d^2}$ becomes of the order one,

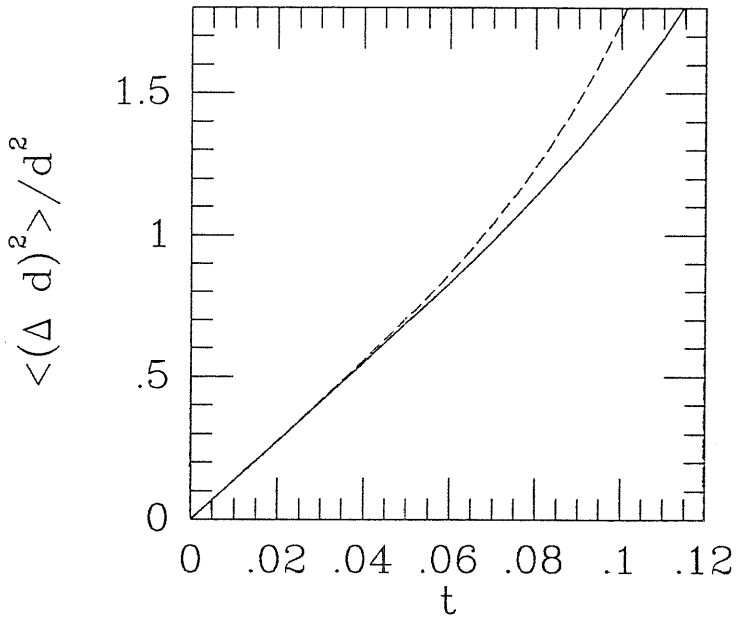

Figure 6.4: Mean square fluctuations of the Flux phase order parameter in presence and absence of the constraint

increases from $t^\star = 0.06$ in absence of the constraint to $t^\star = 0.07$ when the constraint is included.

In conclusion we found that, including gaussian fluctuations and in the whole temperature range in which our mean field solutions are valid, the free energy of the Peierls phase is lower than the Flux phase free energy (Fig.(6.5)).

The effects of the constraint inclusion have been analysed. These mainly consist in an increase of the mean field transition temperature that is the same for both phases and in a depression of the thermal fluctuations around the saddle point solutions that is more remarkable for the Peierls solution (Fig.(6.6)).

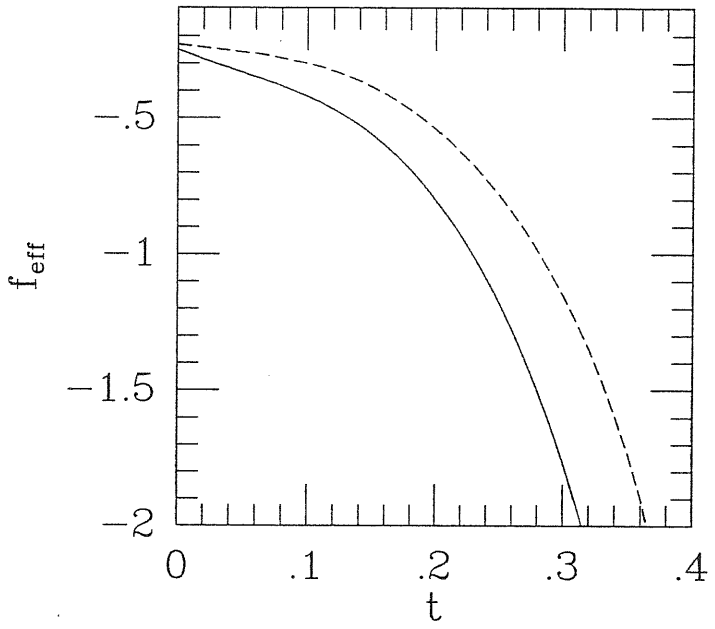

Figure 6.5: Comparison between Peierls (broken curve) and Flux (full curve) phases : the effective free energy vs. reduced temperature

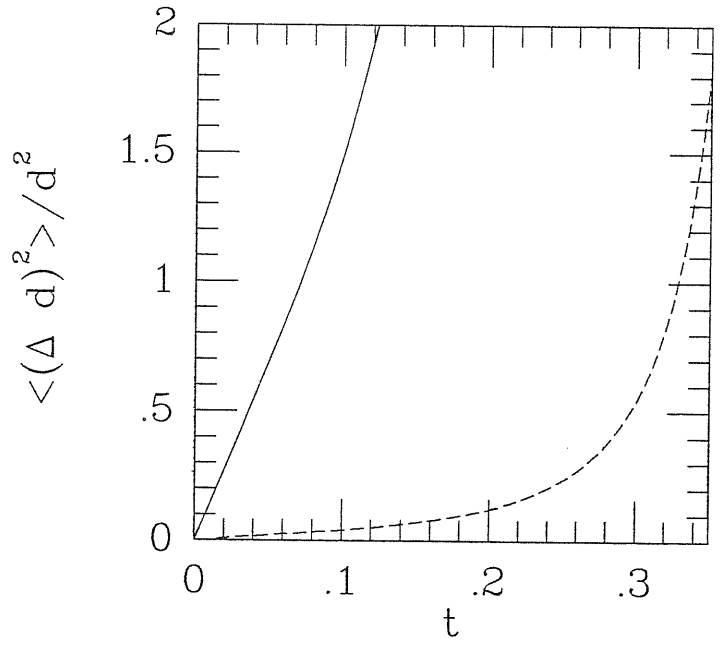

Figure 6.6: Comparison between Peierls (broken curve) and Flux (full curve) phases : Relative mean square fluctuations of the order parameters

7 Extension away from half filling

The superconducting properties of HTCS materials in presence of doping stimulated great effords in the study of the t-J Hamiltonian away from half filling. In this case, antiferromagnetic order is unlikely and many different paramagnetic states have been proposed as good starting points to describe new kind of superconducting states. Here we present the formal extension of our formalism for the partition function incorporating the constraint of no doubly occupied sites.

Moving away from half filling we have to substitute the projector $\mathcal{P} = \prod_i n_i(2 - n_i)$ with the full Gutzwiller projector that is:

$$\mathcal{P} = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow}) \tag{7.1}$$

Also the Heisenberg Hamiltonian must be replaced by the t-J Hamiltonian. The Gutzwiller projector does not commute with the t-J Hamiltonian. Nonetheless, it is still possible to include the constraint operating with functional derivatives on a generating functional which is evaluated as the trace on the complete Hilbert space, so that standard methods can be applied.

Here we discuss one-site projector only to make the notation handly. Let us call this

functional $\mathcal{Z}[z_\uparrow(\tau), z_\downarrow(\tau)]$:

$$\mathcal{Z}[z_\uparrow(\tau), z_\downarrow(\tau)] = Tr\left\{e^{-\beta H} T_\tau e^{-\int_0^\beta d\tau (n_\uparrow(\tau) z_\uparrow(\tau) + n_\downarrow(\tau) z_\downarrow(\tau))}\right\} \tag{7.2}$$

Due to the non commuting property of the projector with the t-J Hamiltonian, we introduce a partition of the imaginary time interval β in N small intervals of "time": $\epsilon = \beta/N$. The time ordered exponential comes from the standard continous generalization used to handle these non commuting terms.

Define the Gutzwiller projector in the interaction rapresentation as:

$$\mathcal{P}(\tau) = e^{\tau H} \mathcal{P} e^{-\tau H} \tag{7.3}$$

that is expilicitely:

$$\mathcal{P} = 1 - n_\uparrow(\tau) n_\downarrow(\tau) \tag{7.4}$$

The partition function:

$$\mathcal{Z} = Tr\left\{\mathcal{P} e^{-\beta H}\right\} \tag{7.5}$$

will be recovered, following the spirit of the half filling case, performing functional derivatives of the generating functional and letting the source fields $z_{\uparrow,\downarrow}(\tau)$ to be equal zero at the end.

The result for the partition function is:

$$\mathcal{Z} = Tr\left\{\mathcal{P} e^{-\beta H}\right\} = \left(1 - \frac{\delta^2}{\delta z_\uparrow(\tau) \delta z_\downarrow(\tau)}\right) \mathcal{Z}[z_\uparrow(\tau), z_\downarrow(\tau)]\Big|_{z_{\uparrow,\downarrow}=0} \tag{7.6}$$

This is the closed formal expression of the partition function that gives the extension of our method away from half filling.

Appendix A
Evaluation of the second derivative of the total effective action

Our starting point is the effective free energy:

$$\beta\mathcal{F}[\mathcal{U}] = N\pi \sum_{i=1}^{4} \mid \mathcal{U} \mid^2 + S_{eff}[\mathcal{U}] - N \ln 4B[\mathcal{U}] \tag{A.7}$$

where, recalling that we defined $x_k = cE(k)$:

$$S_{eff}[\mathcal{U}] = -4 \sum_{k} \ln \cosh \frac{x_k}{2} \tag{A.8}$$

and

$$B = 1 - \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{x_k \tanh x_k/2 - x'_k \tanh x'_k/2}{x_k^2 - x'^2_k} \tag{A.9}$$

The first variation with respect to the fields $\delta\mathcal{U}$ of the effective action term gives:

$$\delta S_{eff} = -cSp\left[\tanh \frac{c\mathcal{U}}{2} \delta\mathcal{U}\right] \tag{A.10}$$

Note that:

$$\tanh\frac{c\mathcal{U}}{2} = -2c\mathcal{U}\sum_n \frac{1}{(i\omega_n)^2 - c^2\mathcal{U}^2} = \tag{A.11}$$

$$= -\sum_n \left(\frac{1}{i\omega_n - c\mathcal{U}} - \frac{1}{i\omega_n + c\mathcal{U}}\right) = -\sum_n (\chi_n^+ - \chi_n^-) \tag{A.12}$$

what defines $\chi^{\pm}$. We can rewrite the variation of the effective action as:

$$\delta S_{eff} = c\sum_n Sp[(\chi_n^+ - \chi_n^-)\delta\mathcal{U}] \tag{A.13}$$

and the constraint contribution as:

$$B = 1 + \sum_n Sp[\chi_n^+ P_i \chi_n^+ P_i + \chi_n^+ P_i \chi_n^- P_i] = 1 + 2\sum_n Sp[\chi_n^+ P_i \chi_n^+ P_i] \tag{A.14}$$

Because is:

$$\delta(\chi_n^{\pm}) = \pm\chi_n^{\pm}\delta\mathcal{U}\chi_n^{\pm} \tag{A.15}$$

the first variation of B reads:

$$\delta B = 4c\sum_n Sp[\chi_n^+ P_i \chi_n^+ P_i \chi_n^+ \delta\mathcal{U}] \tag{A.16}$$

where we have used the permuting properties of the trace. At the end we get:

$$\delta\beta\mathcal{F}_{eff}[\mathcal{U}] = \pi Sp[\mathcal{U}\delta\mathcal{U}] + c\sum_n Sp[(\chi_n^+ - \chi_n^-)\delta\mathcal{U}] - \frac{N}{B}\delta B \tag{A.17}$$

In a similar formal way we have for the second variation of the effective action:

$$\delta^2 S_{eff} = -c^2 \sum_n Sp[\chi_n^+ \delta\mathcal{U} \chi_n^+ \delta\mathcal{U} + \chi_n^- \delta\mathcal{U} \chi_n^- \delta\mathcal{U}] = -2c^2 \sum_n Sp[\chi_n^+ \delta\mathcal{U} \chi_n^+ \delta\mathcal{U}] \qquad (A.18)$$

using the properties: $n \leftrightarrow -n \quad \Rightarrow \quad \chi_n^{\pm} \leftrightarrow \mp\chi_n^{\mp}$. The second variation of B is given by:

$$\delta^2 B = 4c^2 \sum_n 2Sp[\chi_n^+ P_i \chi_n^+ P_i \chi_n^+ \delta\mathcal{U} \chi_n^+ \delta\mathcal{U}] + Sp[\chi_n^+ \delta\mathcal{U} \chi_n^+ P_i \chi_n^+ \delta\mathcal{U} \chi_n^+ P_i] \qquad (A.19)$$

Finally, the complete expression for the second variation of the total effective action per particle, in units of J, is:

$$\delta^2 f_{eff} = 2 \sum_{i=1}^{4} \mid \delta d_i \mid^2 + \frac{t}{N} \delta^2 S_{eff} - t \left(\frac{\delta^2 B}{B} - \frac{(\delta B)^2}{B^2} \right) \qquad (A.20)$$

Performing the Matsubara frequency summations and expressing the traces as sums over the reduced Brilluin zone we get:

$$\sum_{i=1}^{4} \mid \delta d_i \mid^2 = \left(\frac{2}{N} \right) \sum_k \mid \delta d_k \mid^2 \qquad (A.21)$$

$$\frac{t}{N} \delta^2 S_{eff} = 2 \left(\frac{2}{N} \right) \sum_k \left(Q(\mid d_k \mid) \mid \delta d_k \mid^2 + \Re \left[\delta d_k \left(\frac{d_k}{\mid \delta d_k \mid} \right)^2 q(\mid d_k \mid) \delta d_k \right] \right) \qquad (A.22)$$

where:

$$Q(\mid d_k \mid) = -\frac{1}{\mid d_k \mid} \tanh \frac{\mid d_k \mid}{2t} - \frac{1}{8t \cosh^2(\frac{\mid d_k \mid}{2t})} \qquad (A.23)$$

and

$$q(\mid d_k \mid) = \frac{1}{\mid d_k \mid} \tanh \frac{\mid d_k \mid}{2t} - \frac{1}{8t \cosh^2(\frac{|d_k|}{2t})} \tag{A.24}$$

The first variation of the constraint contribution is given by:

$$\delta B = \left(\frac{2}{N}\right)^2 \sum_{k,k'} \left(2\frac{x_k^2 - x_{k'}^2}{(x_k^2 - x_{k'}^2)^2} \tanh x_k/2 - \frac{x_k x_{k'}}{(x_k^2 - x_{k'}^2)^2} \tanh x_{k'}/2 + \right.$$
$$\left. - \frac{x_k}{x_k^2 - x_{k'}^2} \left(1 - \tanh^2 x_k/2\right) \right) A_1 \tag{A.25}$$

Where we have defined:

$$A = A_1 + iA_2 = \frac{1}{t} \left\{ \frac{d_k}{\mid d_k \mid} \delta d_k^* \right\} \tag{A.26}$$

The second variation of the constraint contribution is given, in explicit form, by:

$$\delta^2 B = B_1(A_1 A_1') + B_2(A_1^2) + B_3(A_2^2) \tag{A.27}$$

where A' is a shorthand notation for the k' dependence and

$$B_1(A_1 A_1') = 4 \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{x_k x_{k'}}{(x_k^2 - x_{k'}^2)^2} \left[\frac{(3x_k^2 + x_{k'}^2)}{(x_k^2 - x_{k'}^2)} \frac{2}{x_k} \tanh x_k/2 + \right.$$
$$\left. - \frac{(3x_{k'}^2 + x_k^2)}{(x_k^2 - x_{k'}^2)} \frac{2}{x_{k'}} \tanh x_{k'}/2 - 2 - \tanh^2 x_k/2 - \tanh^2 x_{k'}/2 \right] A_1 A_1' \tag{A.28}$$

$$B_2(A_1^2) = \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{1}{x_k^2 - x_{k'}^2} \left[\frac{-4x_k(x_k^2 + 3x_{k'}^2)}{(x_k^2 - x_{k'}^2)^2} \tanh x_k/2 + \right.$$
$$+ \frac{4x_{k'}(x_{k'}^2 + 3x_k^2)}{(x_k^2 - x_{k'}^2)^2} \tanh x_{k'}/2 + \frac{2(x_k^2 + x_{k'}^2)}{(x_k^2 - x_{k'}^2)} (1 - \tanh^2 x_k/2) +$$
$$\left. + x_k \tanh x_k/2 (1 - \tanh^2 x_k/2) \right] A_1^2 \tag{A.29}$$

$$B_3(A_2^2) = \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{1}{x_k^2 - x_{k'}^2} \left[\frac{2(x_k^2 + x_{k'}^2)}{x_k(x_k^2 - x_{k'}^2)} \tanh x_k/2 + \right.$$
$$\left. - \frac{4x_{k'}}{x_k^2 - x_{k'}^2} \tanh x_{k'}/2 - 1 + \tanh^2 x_k/2 \right] A_2^2 \qquad \text{(A.30)}$$

These complet the evaluation of the second variation of the total effective action.

Appendix B
Zero modes in the Flux phase

We give in this appendix the proof that the second zero mode found in the Flux phase leaves the total effective action unchanged. This zero mode corresponds to:

$$\begin{aligned} d_1 &\rightarrow d\, e^{-i\theta_2} \\ d_3 &\rightarrow d\, e^{i\theta_2} \\ d_{2,4} &\rightarrow d \end{aligned} \tag{B.31}$$

that gives:

$$\frac{\partial \mathrm{d}}{\partial \theta_2} = i\, d \begin{pmatrix} -e^{-i\theta_2} \\ 0 \\ e^{i\theta_2} \\ 0 \end{pmatrix} \tag{B.32}$$

Where $\mid d_k \mid \rightarrow 2\, d\tilde{\epsilon}_k$, with $\tilde{\epsilon}_k = \mid \cos(k_x - \theta_2) - i\cos(k_y) \mid$. We can show analitically that this transformation leaves the free energy unchanged. Knowing that:

$$\delta d_k = \delta(2de^{i\pi/4}(\cos(k_x - \theta_2) - i\cos k_y)) = 2de^{i\pi/4} \sin k_x \delta\theta_2$$

$$= d_k \frac{\sin k_x}{\epsilon_k^2}(\cos k_x + i \cos k_y)\delta\theta_2 \tag{B.33}$$

and considering, for the sake of simplicity, the case in absence of the constraint, we have:

$$\delta^2 S = \frac{4}{N}\sum_k \left(1 + Q + q\Re\left(1 + 2i\cos k_x \frac{(\cos k_x + i\cos k_y)}{\epsilon_k^2}\right)\right)(\delta\theta_2)^2 \tag{B.34}$$

$$= 8d^2(\delta\theta_2)^2 \frac{2}{N}\sum_k \sin^2 k_x \left(1 + Q + q - q\frac{2\cos^2 k_y}{\epsilon_k^2}\right) \tag{B.35}$$

Using the identity:

$$\frac{2}{N}\sum_k \frac{2\cos^2 k_x \cos^2 k_y}{\epsilon_k^2} q = \frac{2}{N}\sum_k Q(2\cos^2 k_x - 1) \tag{B.36}$$

we find:

$$\delta^2 S = 8d^2(\delta\theta_2)^2 \frac{2}{N}\sum_k \left(\frac{1}{2} + (Q - q)\cos^2 k_x\right) \tag{B.37}$$

that is exactly equal to zero due to the gap equation (4.38) which states:

$$\frac{2}{N}\sum_k (Q - q)\cos^2 k_x = -\frac{2}{N}\sum_k \frac{\epsilon_k^2}{2}\frac{1}{2 \mid d_k \mid}\tanh\frac{d\epsilon_k}{t} = -\frac{1}{2} \tag{B.38}$$

Exactly the same proof holds for the other zero mode given by the transformation:

$$\begin{aligned} d_{1,3} &\rightarrow d \\ d_2 &\rightarrow d\, e^{-i\theta_3} \\ d_4 &\rightarrow d\, e^{i\theta_3} \end{aligned} \tag{B.39}$$

that gives:

$$\frac{\partial \mathbf{d}}{\partial \theta_3} = i\ d \begin{pmatrix} 0 \\ -e^{-i\theta_3} \\ 0 \\ e^{i\theta_3} \end{pmatrix} \tag{B.40}$$

Here $d_k \rightarrow 2\ de^{i\pi/4}(\cos(k_x) - i\ \cos(k_y - \theta_3))$, and we can follow the same steps as before only exchanging k_x and k_y.

Appendix C
Diagonalization of the curvature matrix

Results for the Peierls Phase

Here we have $d_k = de^{ik_x}$ and $\mid d_k \mid = d$ and the second variation of the effective free energy, equation (5.5), becomes:

$$\delta^2 f_{eff} = \Gamma \sum_{i=2}^{4} \mid \delta d_i \mid^2 + \Xi \, 2 \left(\Re\{\delta d_1\}\right)^2 \tag{C.41}$$

where

$$\Gamma = 1 - \frac{1}{4t \cosh^2(d/2t)} - \alpha \tag{C.42}$$

$$\Xi = 1 - \frac{1}{4t \cosh^2(d/2t)} - \alpha - \frac{D}{4d} + \frac{D^2}{32t} \tag{C.43}$$

and we have defined:

$$\alpha = \frac{1}{4tB \cosh^2(d/2t)} \left(\frac{1 - 2\sinh^2(d/2t)}{6 \cosh^2(d/2t)} + \frac{t^2}{d^2}(1 - \frac{t}{d}\sinh(d/2t)) \right) \tag{C.44}$$

and $D = \frac{\partial}{\partial(d/t)} \ln B$. When D is neglected this is a generalization of the AM result to finite temperature. The quadratic part of the action is written in the basis: $(\delta d_1, \delta d_1^\star, \delta d_2, \delta d_2^\star, \delta d_3, \delta d_3^\star, \delta d_4, \delta d_4^\star)$ and in this case we have a matrix in block form :

$$M = \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \tag{C.45}$$

where

$$M_1 = \begin{pmatrix} a & b \\ b & a \end{pmatrix} \tag{C.46}$$

with $a = \Gamma$ and $b = \Xi$ while the matrix M_2 is a 6X6 diagonal matrix with all the diagonal elements equal to a. The eigenvalues are $\lambda_1 = a$, six times degenerate , $\lambda_2 = a + b$ and $\lambda_3 = 0$. When B is taken to be 1, we have $\lambda_1 = 1 + Q$ six times degenerate, $\lambda_2 = 1 + Q + q = 2\lambda_1$ and $\lambda_3 = 1 + Q - q = 0$ due to the gap equation (5.10). In both cases this zero eigenvalue comes from the residual gauge invariance that leaves the phase of d_1 undetermined. This can be easily seen in absence of the constraint when Γ and Ξ coincide so that the imaginary part of d_1 disappears from the equation (C.41). It is useful and easy to check the calculation trough the limit of λ_i as $t \to t_c$ that must be zero because the free energy becomes flat at that temperature around the mean field solution.

The same procedure can be repeated in presence of the constraint with the only difference that now the functions a and b are changed. In the same way one zero eigenvalue is obtained. As the same as in the previous case one can show analitically that λ_3 is zero using the self consistency equation for the order parameter (Appendix B).

Results for the Flux Phase

Here we have:

$$d_k = 2d(\cos k_x - i \cos k_y) \quad ; \quad \mid d_k \mid = 2d\epsilon_k = 2d\sqrt{\cos^2(k_x) + \cos^2(k_y)} \tag{C.47}$$

From the equation (5.5) we can isolate three contributions to the second variation of the effective free energy which reads:

$$\delta^2 f_{eff} = \frac{2}{N} \sum_k \left(A_k \mid \delta d_k \mid^2 + B_k \Re \left\{ \delta d_k \frac{d_k^{\star 2}}{\mid d_k \mid^2} \delta d_k \right\} \right) + \\ + C \sum_{i,j} (\delta d_i + \delta d_i^\star) \Gamma_{ij} (\delta d_i + \delta d_i^\star) \tag{C.48}$$

where:

$$A_k = 1 + Q_k - \frac{t}{2B} (\Psi_1(k) + \Psi_2(k)) \tag{C.49}$$

$$B_k = q_k - \frac{t}{2B} (\Psi_1(k) - \Psi_2(k)) \tag{C.50}$$

$$C = -\frac{t}{2B} \left(\Xi - \frac{\Upsilon}{B} \right) \tag{C.51}$$

and we have defined

$$\Psi_1(k) = \left(\frac{2}{N} \right) \sum_{k'} \frac{1}{4d^2(\epsilon^2 - \epsilon'^2)^2} \left[-\frac{t}{d} \frac{\epsilon(3\epsilon'^2 + \epsilon^2)}{(\epsilon^2 - \epsilon'^2)^2} \tanh(\frac{d\epsilon}{t}) + \right. \\ + \frac{t}{d} \frac{\epsilon'(3\epsilon^2 + \epsilon'^2)}{(\epsilon^2 - \epsilon'^2)^2} \tanh(\frac{d\epsilon'}{t}) + \frac{\epsilon^2 + \epsilon'^2}{\epsilon^2 - \epsilon'^2} \left(1 - \tanh^2(d\epsilon/t) \right) + \\ \left. + \frac{d\epsilon}{t} \tanh(d\epsilon/t) \left(1 - \tanh^2(d\epsilon/t) \right) \right] \tag{C.52}$$

$$\Psi_2(k) = \left(\frac{2}{N}\right) \sum_{k'} \frac{1}{4d^2(\epsilon^2 - \epsilon'^2)} \left[\frac{t}{2d} \frac{\epsilon'^2 + \epsilon^2}{\epsilon(\epsilon^2 - \epsilon'^2)} \tanh(\frac{d\epsilon}{t}) + \right.$$
$$\left. - \frac{t}{d} \frac{\epsilon'}{(\epsilon^2 - \epsilon'^2)} \tanh(\frac{d\epsilon'}{t}) + \frac{1}{2} \left(1 - \tanh^2(d\epsilon/t)\right) \right] \quad \text{(C.53)}$$

$$\Xi = \left(\frac{2}{N}\right)^2 \sum_{k,k'} \frac{\epsilon\epsilon'}{16d^2(\epsilon^2 - \epsilon'^2)^2} \left[\frac{t}{d} \frac{3\epsilon^2 + \epsilon'^2}{\epsilon(\epsilon^2 - \epsilon'^2)} \tanh(\frac{d\epsilon}{t}) + \right.$$
$$\left. - \frac{t}{d} \frac{3\epsilon'^2 + \epsilon^2}{\epsilon'(\epsilon^2 - \epsilon'^2)} \tanh(\frac{d\epsilon'}{t}) - 2 + \tanh^2(\frac{d\epsilon}{t}) + \tanh^2(\frac{d\epsilon'}{t}) \right] \quad \text{(C.54)}$$

$$\Upsilon = (\delta B)^2 \quad \text{(C.55)}$$

We can define the only different matrix elements:

$$\begin{aligned}
a_1 &= \frac{2}{N} \sum_k A_k + C \\
a_2 &= \frac{2}{N} \sum_k A_k(\cos^2 k_x - \sin^2 k_x) + C \\
b_1 &= \frac{2}{N} \sum_k 2B_k \left(\frac{\cos^4 k_x - \cos^2 k_x \cos^2 k_y}{\epsilon_k^2} \right) - C \\
b_2 &= \frac{2}{N} \sum_k 2B_k \frac{\cos^2 k_x \cos^2 k_y}{\epsilon_k^2} + C \\
c &= C
\end{aligned} \quad \text{(C.56)}$$

The final matrix in the vector base $(\delta d_1^\star, \delta d_2, \delta d_3^\star, \delta d_4, \delta d_1, \delta d_2^\star, \delta d_3, \delta d_4^\star)$ is given by:

$$M = \begin{pmatrix} a_1 & -ic & a_2 & -ic & ib_1 & b_2 & -ic & b_2 \\ ic & a_1 & ic & a_2 & b_2 & -ib_1 & b_2 & ic \\ a_2 & -ic & a_1 & -ic & -ic & b_2 & ib_1 & b_2 \\ ic & a_2 & ic & a_1 & b_2 & ic & b_2 & -ib_1 \\ -ib_1 & b_2 & ic & b_2 & a_1 & ic & a_2 & ic \\ b_2 & ib_1 & b_2 & -ic & -ic & a_1 & -ic & a_2 \\ ic & b_2 & -ib_1 & b_2 & a_2 & ic & a_1 & ic \\ b_2 & -ic & b_2 & ib_1 & -ic & a_2 & -ic & a_1 \end{pmatrix} \tag{C.57}$$

This matrix turn out to be centrosymmetric and its determinant can be reduced to the product of two 4X4 determinats. After some algebra one can find the eigenvalues:

$$\begin{aligned} \lambda_1 &= a_1 - a_2 - b_1 - c \\ \lambda_2 &= a_1 - a_2 + b_1 + c \\ \lambda_3 &= a_1 + a_2 + b_1 + 2b_2 - 3c \\ \lambda_4 &= a_1 + a_2 - b_1 + 2b_2 + 3c \end{aligned} \tag{C.58}$$

λ_1 is three times degenerate and can be proved to be equal zero. λ_2 also is three times degenerate.

Appendix D
Zero modes integration

In order to calculate the gaussian correction to the free energy we have to identify the zero modes. Then we can apply the standard Fadeev-Popov procedure to integrate out these zero modes and perform the usual gaussian integration on the collective modes described previously. The standard precedure runs as follows. Given the original path integral:

$$e^{-\beta \mathcal{F}_{eff}} = e^{-\beta \mathcal{F}^0_{eff}} \prod_{ij} \int d^2\delta d_{ij} e^{-\pi \delta d^* M' \delta d} \tag{D.59}$$

that we can rewrite, using the chosen symmetries for the 2N bonds variables, as:

$$\prod_{ij} \int d^2\delta d_{ij} e^{-\pi \delta d^* M' \delta d} = \left[\prod_{i=1}^{4} \int d^2\delta d_i e^{-\pi \delta d^* M' \delta d} \right]^{\frac{N}{2}} \tag{D.60}$$

In the general case we can define the projection of the curvature matrix M' on the subspace orthogonal to the zero modes: $M'_\perp$. In block matrix form we have:

$$M' = \begin{bmatrix} 0 & 0 \\ 0 & M'_\perp \end{bmatrix} \tag{D.61}$$

The standard integration procedure[41], when the zero modes $\frac{\partial \mathbf{d}}{\theta_i}$ have been identified, gives:

$$\mathcal{Z} = e^{-\beta \mathcal{F}^0_{eff}} \frac{1}{\sqrt{det M'_\perp}} \int \prod_{i=1}^{n} \frac{d\theta_i}{\sqrt{2\pi}} (det \mathcal{N})^{1/2} \tag{D.62}$$

the matrix $\mathcal{N}$, whose dimension is given by the number of zero modes, has elements given by:

$$\mathcal{N}_{ij} = \sum_{l=1}^{8} \frac{\partial d_l{}^\star}{\partial \theta_i} \cdot \frac{\partial d_l}{\partial \theta_j} \tag{D.63}$$

The only zero mode present in the Peierls phase corresponds to:

$$\begin{aligned} d_{1,3} &\rightarrow d\, e^{i\theta_1} \\ d_{2,4} &\rightarrow d\, e^{-i\theta_1} \end{aligned} \tag{D.64}$$

that gives:

$$\frac{\partial \mathbf{d}}{\partial \theta_1} = i\, d \begin{pmatrix} e^{i\theta_1} \\ -e^{-i\theta_1} \\ e^{i\theta_1} \\ -e^{-i\theta_1} \end{pmatrix} \tag{D.65}$$

Here we have $d_k \rightarrow d_k e^{i\theta}$.

For the flux phase we found three zero modes, one is the above described and the second one corresponds to:

$$\begin{aligned} d_1 &\rightarrow d\, e^{-i\theta_2} \\ d_3 &\rightarrow d\, e^{i\theta_2} \\ d_{2,4} &\rightarrow d \end{aligned}$$

(D.66)

that gives:

$$\frac{\partial \mathbf{d}}{\partial \theta_2} = i\ d \begin{pmatrix} -e^{-i\theta_2} \\ 0 \\ e^{i\theta_2} \\ 0 \end{pmatrix} \tag{D.67}$$

Where $\mid d_k \mid \rightarrow 2\ d\tilde{\epsilon}_k$, with $\tilde{\epsilon}_k = \mid \cos(k_x - \theta_2) - i\cos(k_y) \mid$.

The third transformation is given by:

$$\begin{aligned} d_{1,3} &\rightarrow d \\ d_2 &\rightarrow d\ e^{-i\theta_3} \\ d_4 &\rightarrow d\ e^{i\theta_3} \end{aligned} \tag{D.68}$$

that gives:

$$\frac{\partial \mathbf{d}}{\partial \theta_3} = i\ d \begin{pmatrix} 0 \\ -e^{-i\theta_3} \\ 0 \\ e^{i\theta_3} \end{pmatrix} \tag{D.69}$$

Here $d_k \rightarrow 2\ de^{i\pi/4}(\cos(k_x) - i\ \cos(k_y - \theta_3))$.

It is worth noticing that we used a basis $(\delta d_1, \delta d_1^\star, \delta d_2, \delta d_2^\star, \delta d_3, \delta d_3^\star, \delta d_4, \delta d_4^\star)$, because the gauge transformations and the zero modes turn out to be of much more clear physical interpretation.

However, the path integral we want to perform is over the real and imaginary parts of the d_i fields. In order to apply equation (6.7) we have to transform $\frac{\partial \mathbf{d}}{\partial \theta}$ to the basis of real and imaginary parts of the d_i. Doing that we get:

$$\frac{\partial \mathbf{d}}{\partial \theta_1} \rightarrow$$

$$(-\sin\theta_1, -\sin\theta_1, -\sin\theta_1, -\sin\theta_1, i\cos\theta_1, -i\cos\theta_1, i\cos\theta_1, -i\cos\theta_1)$$

$$\frac{\partial \mathbf{d}}{\partial \theta_2} \rightarrow$$

$$(-\sin\theta_2, 0, -\sin\theta_2, 0, -i\cos\theta_2, 0, -i\cos\theta_2, 0)$$

$$\frac{\partial \mathbf{d}}{\partial \theta_3} \rightarrow$$

$$(0, -\sin\theta_3, 0, -\sin\theta_3, 0, -i\cos\theta_3, 0, -i\cos\theta_3) \tag{D.70}$$

(D.71)

For the Peierls phase the final result is:

$$f^{eff} = f_0^{eff} - \frac{t}{2}\ln\left(\frac{d^2}{\sqrt{\prod_i' \lambda_i}}\right) \tag{D.72}$$

For the flux phase, the matrix elements of $\mathcal{N}$ are:

$$\begin{aligned}
\mathcal{N}_{11} &= 4d^2 \\
\mathcal{N}_{22} &= 2d^2 \\
\mathcal{N}_{33} &= 2d^2 \\
\mathcal{N}_{12} &= 2d^2 \sin\theta_1 \sin\theta_2 \\
\mathcal{N}_{13} &= 2d^2 \sin\theta_1 \sin\theta_3 \\
\mathcal{N}_{23} &= 0
\end{aligned} \tag{D.73}$$

and:

$$det\mathcal{N} = (2d^2)^3(2 - \sin^2\theta_1 \sin^2\theta_2 - \sin^2\theta_1 \sin^2\theta_3) \tag{D.74}$$

so that after integrating over the angular variables we get the final result:

$$f_{eff} = f^0_{eff} - \frac{t}{2}\ln\left(\frac{(2d^2)^{3/2}1.203}{\sqrt{\prod_i' \lambda_i}}\right) \tag{D.75}$$

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