Fermionic linearization for systems of itinerant interacting electrons

Thesis presented by

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Introduction

The recent discovery of high-T_c superconducting materials [11] has revived the interest in the physics of strongly correlated systems. In fact these ceramic superconductors are good insulators, and on the other hand, expecially in the CuO_2 two-dimensional planes in which superconductivity takes place, they can exhibit strong antiferromagnetic correlations, with the antiferromagnetic phase remarkably close to the superconducting one. Therefore, the relevance of the interplay between magnetic behavior and metal-insulator transition (also known as *Mott transition*) near half-filling seems to be crucial.

The simplest model to describe the main features of strongly correlated electrons is the so-called Hubbard model, originally introduced in [40] as an attempt to describe the effect of correlations for d-electrons in transition metals. The model hamiltonian consists of two contributions,

$$H = - \sum_{<i,j>} \sum_{\sigma} t_{ij} (a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \quad , \qquad (0.1)$$

a kinetic term describing the motion of electrons between neighbouring sites (the hopping integral $t_{i,j}$ is usually restricted to nearest-neighbours) and a on-site term, which approximates the interactions among electrons. The indices i, j label the sites of a d-dimensional lattice Λ.

A considerable amount of work has been devoted to the solution of the Hubbard model since its introduction in physics. The limits $t \to 0$ (fully localized electrons) and $U \to 0$ (free itinerant electrons) yield hamiltonians solvable in any dimension. For intermediate couplings, the model is not exactly solvable, except in one dimension where it has been solved by Lieb and Wu [47], using the Bethe Ansatz technique. In the latter case, however, the Mott transition is absent at any $T \neq 0$, according to the Mermin-Wagner theorem.

The failure of exact results in dimensions greater than one has naturally stimulated the growth of several approximation methods [50, 38], particularly in the limit

$|U/t| \to \infty$ (strong-coupling regime) and in proximity of band half-filling, where analytical methods and numerical simulations have answered a lot of questions about the magnetic behavior of the model. [1]

However, it is still not clear if the Hubbard model itself is capable of describing a superconducting phase, [2] therefore extensions of the model have been proposed to enhance this possibility. The simplest choice consists in adding to the Hubbard model coulomb interactions between nearest-neighbour sites of the form $\sum_{<ij>} \sum_{\sigma\sigma'} V_{ij} n_{i\sigma} n_{j\sigma'}$, resulting in what is referred to as the *extended Hubbard model*. Furthermore, the neighborood of antiferromagnetism (AF) and superconductivity (SC) in the phase diagram of the high-T_c cuprates indicates that AF correlations may play an important role in the pairing mechanism. Now, the starting point for all the schemes proposed so far which involve AF interactions is a more or less large on-site Coulomb repulsion energy U_d on the Cu d-orbitals considered usually within the frame of the single-band Hubbard model in two dimensions. While the corresponding large U limit of this single-band Hubbard model is indeed in accord with some essential magnetic properties of the CuO materials at half-filling [19], there is a growing evidence that a multiband Hubbard model is required to account for charge fluctuations, and spetroscopic data clearly point to the necessity to consider both Cu-$3d$ and O-$2p$ orbitals together with their intra- and interatomic correlations. Therefore, many studies have been done on this three-band extended Hubbard model [74, 64, 34].

Among the various approaches to models describing interacting many- fermions systems, a particular method has been introduced by Solomon [70, 71]. The strategy adopted there amounts essentially to linearizing the hamiltonian by a mean-field approximation, which leads to a conventional pair-reduced mean-field model. The effective hamiltonian is then recognized to be an element (of a representation) of a Lie algebra $\mathcal{A}$, referred to as the spectrum-generating algebra (SGA); through an automorphism of $\mathcal{A}$, it is then possible to diagonalize the hamiltonian, leading to the energy spectrum. Finally, self-consistency equations reconduct the exact results for the linearized model to approximate (mean-field like) results for the original model.

The use of SGA's permits a unified treatment of systems exhibiting coexistence of competing order parameters such as superconductivity, charge density waves and spin density waves [15] and the construction of the many fermion Green function for $T = 0$ and $T \neq 0$ from factors completely determined by the underlying dynamical

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[1] We refer to [41], where the most important articles related to this topic are contained

[2] Some people believe that the Hubbard model could describe d-wave SC but high-T_c materials also show s-wave SC

algebra [13].

In [53], a refinement of the Solomon's method, called successively *fermionic linearization* has been proposed. It is characterized by the fact that expectation values of fermionic operators to be self-consistently evaluated in the ground state (or in some suitable equilibrium quantum state) must be taken as odd elements of a Grassmann-like algebra $\mathcal{G}$, anticommuting among themselves and with the fermionic operators.

The Hubbard model, when fermi-linearized, exhibits a dynamical algebra which is a *superalgebra* (also called $\mathbb{Z}_2$-graded algebra). This is also the case for an extension of the model to a superlattice consisting of the sum of two sublattices , when dealt with in a generalized mean-field scheme where a cluster of two sites is treated exactly instead of a single site [54]. Based on these results, supersymmetric hamiltonians has been constructed from conserved fermionic charges living in the fermionic sector of the superalgebra. The resulting hamiltonians are then generalizations of the Hubbard model, exhibiting superconductive-magnetic phase whose appearance is associated with spontaneous supersymmetry breaking.

Furthermore, it is interesting to point out that the structure of the superlattice realizing the supersymmetry is indeed that of most of the known compounds exhibiting high-T_c SC. For this reason it seems reasonable to suggest the hypothesis that spontaneous supersymmetry breaking could be a possible mechanism to account for high-T_c superconductive phase transition in systems, such as the ceramic rare earth doped copper oxides, well described by Hubbard-like hamiltonians.

This thesis is devoted to the application of the fermi-linearization scheme to Hubbard-like models and is fundamentally divided into two parts. The first part composed by the first two chapters includes a review of the known results. The second part, composed by chapter 3 and 4, contains the original results recently published in [20, 21, 22, 52]. The work is completed, as usual, with the conclusions and the outlooks.

In Chapter 1, we introduce the concept of dynamical algebra of a system, giving the various choices for the Grassmann-like algebra related to fermionic linearization. We also show how order operators in Hilbert space can be associated to elements of the SGA. Then we illustrate the SGA method with the conventional linearized BCS model and with a more complex system of interacting fermions showing the coexistence of three phases. The chapter is closed showing how the BCS model, when fermi-linearized, may be regarded as the hamiltonian of a model exhibiting spontaneously symmetry breaking.

Chapter 2 is completely devoted to the fermi-linearized Hubbard model. The

Grassmann-like algebra will be here a Banach-Grassmann algebra. First, we describe the model, showing the connections with high-T_c superconductivity. Then, we show the possible breakings of the SO(4) symmetry discovered by Yang and Zhang, with the related order parameters. Here, the difference between fermionic linearization scheme and other approximation methods is pointed out. After a general analysis of the dynamical superalgebra for the n-cluster fermi-linearized Hubbard model, we then study the thermodynamics in the case $n = 1$ (single-site) and the ground state for the case $n = 2$ (dimer). The last section contains a discussion about the supersymmetric extensions of the Hubbard model in two dimensions previously mentioned.

Chapter 3 is entirely dedicated to a particular version of the extended Hubbard model called the extended Falicov-Kimball model [20, 21]. Partition function and self-consistency equations are derived in details. Then a special solution of the problem is presented together with numerical results. Also in this case, a Banach Grassmann algebra has been used.

Chapter 4 deals with the case where the Grassmann-like algebra is a Clifford algebra. The dynamical algebras for the Hubbard and the extended Hubbard models, which in this case are no longer superalgebras but ordinary Lie algebras, are derived [22, 23]. We give a numerical analysis for the Falicov-Kimball [52].

Those who are not familiar with concepts like Lie algebras, superalgebras, supersymmetry and coherent states can look at the appendices where a short introduction to these notions is contained.

Chapter 1

The Fermi-linearization scheme

1.1 Dynamical groups and coexistence phenomena

The relationship between symmetry groups and phase transitions is well-known: the transition of a system from one phase to another is usually accompagnied by the spontaneous breaking of the symmetry group G associated with the system. That is, the latter in its disordered state (above a critical temperature T_C) , is described by a Hamiltonian H having symmetry group G, whence in the ordered state (below T_C), it is described by a reduced hamiltonian H_{red} which is invariant under a smaller symmetry group $G_0 \subset G$. The appearance of order parameters will then be associated to the disappearance of the higher symmetry.

Well-known cooperative many-body effects such as superconductivity, charge- and spin-density waves, ferromagnetism, etc. can be investigated as broken symmetries. For example, above T_C, a ferromagnet is rotationally invariant and $G = SO(3)$. Below T_C, an arbitrary but fixed direction in direct space is distinguished. The axis of the magnetization $\mathbf{M} \neq 0$, which in this case is the order parameter, becomes the axis of lower symmetry and $G_0 = SO(2)$. For a superconductor, one assumes that above T_C, the fields satisfy angle-phase $(U(1))$ invariance (equivalent, by Noether's theorem, to number conservation). In the superconducting state, this $U(1)$ invariance is broken. In this case, the order parameters are the fields or their expectation values if quantum theory is used.

The discovery of the presence of coexisting phases in certain alloys at low temperatures ([73]) raised the question whether the general coexistence problem of many-fermion systems can be suitably handled in a compact way within a unified group theoretical approach.

In this context, the concept of *dynamical group* has been introduced [70]. Dynamical groups, which describe both the symmetry of the system and its spectrum, arise in the following way: the reduced hamiltonian, usually a mean-field approximation, is a representation of an element of a Lie algebra, the so-called Spectrum Generating Algebra (SGA). The name of the algebra derives from its property of generating the spectrum of the system, and the dynamical group is usually defined as the Lie group of this SGA.

1.2   The linearization procedure

In this thesis, we will be primarily concerned with hamiltonians describing systems of interacting fermions:

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \frac{1}{2} \sum_{ijkl} < i,j \mid V \mid k,l > a_i^\dagger a_j^\dagger a_k a_l. \tag{1.1}$$

where the label i is a multi-index including both momentum and spin indices ($i \equiv (k,\sigma)$). As usual, $a_i^\dagger, a_i$ are creation and annihilation operators of fermions in the state labelled by the index i satisfying $\{a_i, a_j\} = 0$, $\{a_i, a_j^\dagger\} = \delta_{ij}$.

Methods of solution which we will refer to as linearization methods usually involve the reduction of the four-fermions term in the interaction to multilinear terms of lower order or the linearization of the kinetic term, leading to a reduced Hamiltonian H_{MF} which is expressed as a linear combination of multilinear products of fermion operators. The closure, under Lie bracket, of these multilinears generates then the SGA of that hamiltonian.

From a general point of view, let us consider the product of two operators A and B, and write the identity

$$AB = (A- <A>)(B- <B>)+ <A> B + A <B> - <A><B> . \tag{1.2}$$

where $<A>, <B>$ are the expectation values of the respective operators A and B in some suitable equilibrium quantum state or statistical mechanical average. If we assume that the terms $(A- <A>)$ and $(B- <B>)$ are "small", their product can be neglected and the above identity is replaced by the approximate expression

$$AB \simeq <A> B + A <B> - <A><B> . \tag{1.3}$$

At this point, in order to keep consistency, we have two possibilities which we shall discuss in the following two subsections.

1.2.1 Bosonic linearization

The operators A and B in (1.3) commute: then BA leads to the same linear approximation of AB with < A > and < B > ordinary c-numbers.

In this case, typically, A and B are identified successively with all different pairs of commuting operators entering the four-fermions interaction and use of the approximate identity (1.3) transforms H into a bilinear form, which belongs to an ordinary Lie algebra. We mention, as well-known representative examples, *Hartree, Hartree-Fock, and BCS* approximations. For further purposes, we give below the algebras related to single and pair fermion operators.

Algebras for fermion operators

We consider a fermion system with N single particle states, labelled by indices $\alpha, \beta, \gamma, \dots$, etc. We define the pair operators of the fermions by

$$
\begin{aligned}
E^\alpha_\beta &= a^\dagger_\alpha a_\beta - \frac{1}{2}\, \delta_{\alpha\beta} \quad, \\
E_{\alpha\beta} &= a_\alpha a_\beta, \quad E^{\alpha\beta} = a^\dagger_\alpha a^\dagger_\beta
\end{aligned}
\tag{1.4}
$$

with the properties $E^{\alpha\dagger}_\beta = E^\beta_\alpha, E^{\alpha\beta} = E^\dagger_{\beta\alpha}, E_{\alpha\beta} = -E_{\beta\alpha}$. The set consisting of all single and pair operators generates the Lie algebra B_N isomorphic to $so(2N+1)$. The commutation relations are given by:

$$
\begin{aligned}
[\, E^\alpha_\beta, E^\gamma_\delta\,] &= \delta_{\gamma\beta} E^\alpha_\delta - \delta_{\alpha\delta} E^\gamma_\beta \quad, \\
[\, E^\alpha_\beta, E_{\gamma\delta}\,] &= \delta_{\alpha\delta} E^{\beta\gamma} - \delta_{\alpha\gamma} E_{\beta\delta} \quad, \\
[\, E^{\alpha\beta}, E_{\gamma\delta}\,] &= \delta_{\alpha\delta} E^\beta_\gamma + \delta_{\beta\gamma} E^\alpha_\delta - \delta_{\alpha\gamma} E^{\beta\delta} - \delta_{\beta\delta} E^\alpha_\gamma \quad, \\
[\, E_{\alpha\beta}, E_{\gamma\delta}\,] &= 0 \quad, \\
[\, a^\dagger_\alpha, a_\beta\,] &= 2\, E^\alpha_\beta, \quad [\, a_\alpha, a_\beta\,] = 2\, E_{\alpha\beta}, \\
[\, a_\alpha, E^\beta_\delta\,] &= \delta_{\alpha\beta} a_\gamma, \quad [\, a_\alpha, E_{\beta\delta}\,] = 0 \quad, \\
[\, a_\alpha, E^{\beta\delta}\,] &= \delta_{\alpha\beta} a^\dagger_\gamma - \delta_{\alpha\gamma} a^\dagger_\beta \quad.
\end{aligned}
\tag{1.5}
$$

The other commutators are straightforwardly obtained by hermitian conjugation. From (1.5), the set of all pair operators (1.4) is closed under commutation and generates the algebra $D_N \sim so(2N)$, while the subset $\{E^\alpha_\beta\}$ forms a $u(N)$ Lie algebra.

1.2.2 Fermionic linearization

The operators A and B anticommute: then $< A >, < B >$ should anticommute with the operators A, B and among themselves.

In this approach, we linearize the hopping term in the following way:

$$\sum_{<i,j>} a^{\dagger}_{i,\sigma} a_{j,\sigma} \rightarrow q \sum_{i} (< a^{\dagger}_{i\sigma} > a_{j\sigma} + a^{\dagger}_{i,\sigma} < a_{j\sigma} > - < a^{\dagger}_{i\sigma} >< a_{j\sigma} >) \quad , \qquad (1.6)$$

where q denotes the number of nearest neighbours per site in the lattice.

For the four-fermions interaction term, the linearization will proceed by replacing

$$a^{\dagger}_i a^{\dagger}_j a_k a_l \rightarrow < a^{\dagger}_i a^{\dagger}_j a_k > a_l + a^{\dagger}_i a^{\dagger}_j a_k < a_l > - < a^{\dagger}_i a^{\dagger}_j a_k >< a_l > . \qquad (1.7)$$

Let us now notice that if this linearization procedure is applied to the hamiltonian (1.1), it can never happen that A equals B or $B^{\dagger}$ and therefore we have no constraints on $< A >< A >^*$ and $< B >< B >^*$. This means that we have various choices for the algebraic object to incorporate $< A >$ and $< B >$ and achieve the above condition. Let us define the numbers $\Theta_i \equiv < A_i >$, where A_i could be a linear or a trilinear in fermion operators, then the Θ_i may belong to:

1. **Grassmann algebra** [1]: a Grassmann algebra $\mathcal{G}$ has a $\mathbb{Z}_2$-gradation in two non-intersecting subsets of elements which are products of even ($\mathcal{G}_0$) and odd ($\mathcal{G}_1$) numbers of anticommuting objects, respectively, that is $\mathcal{G} = \mathcal{G}_0 \oplus \mathcal{G}_1$, with $[\mathcal{G}_0, \mathcal{G}_1] = 0$. The (anti)commutation relations are given by

$$\{\Theta_i, \Theta_j\} = 0 \quad , \quad \{\Theta_i, \bar{\Theta}_j\} = 0 \quad . \qquad (1.8)$$

   We will not consider this possibility, because, due to the associativity, quantities like $(\bar{\Theta}\Theta)^2$ vanish and this fact makes it difficult to give to results of computations inside the algebra, a sound physical interpretation.

2. **Non-associative Banach-Grassmann algebra**: it has the same structure and algebraic relations (1.8) of the Grassmann algebra plus a set of new relations implying that bilinears of the type $\Theta_i \bar{\Theta}_j$ are c-numbers. Therefore, since $(\bar{\Theta}\Theta) = c$ $(c \in \mathbb{R})$, $(\bar{\Theta}\Theta)^2 = c^2$. In the reduced hamiltonian we will then have coefficients at most linear in the variables $\Theta, \bar{\Theta}$. A possible realization could be $\Theta_i \Theta_j \sim \sin(\varphi_i - \varphi_j)$.

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[1] See appendix B for a more detailed definition

3. **Clifford algebra:** the (anti)commutation relations are now

$$\{\Theta_i, \Theta_j\} = 0 \quad , \quad \{\Theta_i, \bar{\Theta}_j\} = \delta_{ij} \quad . \tag{1.9}$$

In the following, we will generally denote by Grassmann-like algebras the group of three algebras introduced right now. Chapter 2 and 3 will be devoted to the case (2), while case (3) will be the subject of Chapter 4.

1.3 The algebraic structure

1.3.1 The Cartan-Weyl basis

In general, for a rank-l, d-dimensional semi-simple Lie algebra g, [2] we may choose the Cartan-Weyl (CW) basis

$$\{h_1, \ldots, h_l; e_{\pm 1}, \ldots, e_{\pm m}\}, \quad l + 2m = d \tag{1.10}$$

where

$$[h_i, h_j] = 0, \quad [h_i, e_{\pm \alpha}] = \pm \alpha_i e_\alpha$$

$$[e_\alpha, e_\beta] = N_{\alpha\beta} e_{\alpha+\beta} \quad (\alpha + \beta \neq 0) \tag{1.11}$$

$$[e_\alpha, e_{-\alpha}] = \sum_{i=1}^{l} \alpha_i h_i.$$

If g is the SGA, we can rewrite H_{MF} in the CW-basis as follows:

$$H_{MF} = \sum_{j=1}^{l} \beta_j \, h_j + \sum_{\alpha=1}^{m} \mu_\alpha (e_\alpha + e_{-\alpha}). \tag{1.12}$$

1.3.2 Bogoliubov transformation

H_{MF} can be rotated to diagonal form by means of an automorphism $\Phi : g \rightarrow g$ represented here by the adjoint action of the operator $Z = \sum_{\alpha=1}^{m} \phi_\alpha (e_\alpha - e_{-\alpha})$. By diagonal we mean that $\mathcal{H}_D = \exp(\text{ad } Z)(H_{MF})$, through an appropriate choice of the coefficents $\{\phi_\alpha\}$, will belong to the commuting Cartan subalgebra generated by the set $\{h_i\}$.

The diagonalization is performed in the following way. First notice that

$$\mathcal{H} = \exp(\text{ad } Z)(H_{MF}) = \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{[Z, \ldots, [Z, H_{MF}] \ldots]}_{n-\text{times}} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} H^{(n)} \quad . \tag{1.13}$$

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[2]See appendix A

Due to the fact that $[Z, H_{MF}] \in g$, we can generally write

$$H^{(k)} = [Z, H^{(k-1)}] = \sum_{j=1}^{l} \beta_j^{(k)} \, h_j + \sum_{\alpha=1}^{m} \mu_\alpha^{(k)}(e_\alpha + e_{-\alpha}), \qquad (1.14)$$

with $H^{(0)} \equiv H_{MF}$, and the commutator defines a recursive relation for the coefficients $\{\beta_j^{(k)}, \mu_\alpha^{(k)}\}$.

Now let us introduce the vector $\mid v >^{(k)} = \mid \mu_1^{(k)}, \ldots, \mu_m^{(k)}, \beta_1^{(k)}, \ldots, \beta_1^{(l)} >$, $l + m = p$ together with $\mid \mathcal{G} >= \mid \hat{e}_1, \ldots, \hat{e}_m, h_1, \ldots, h_l >$, $\hat{e}_\alpha \equiv e_\alpha + e_{-\alpha}$, in such a way that $H^{(k)} =< v^{(k)} \mid \mathcal{G} >$. It is then possible to write down a $p \times p$ matrix A such that $\mid v >^{(k+1)} = A \mid v >^{(k)}$ where $A = A(\{\phi_\alpha\})$ and

$$A_d = T^{-1} A T = \text{diag} \, (\lambda_1, \ldots, \lambda_p). \qquad (1.15)$$

Defining by $\mid \omega >\equiv (\, \nu_1, \ldots, \nu_m, \gamma_1, \ldots, \gamma_l)$ the coefficients relative to $\mathcal{H}$, (i.e. $\mathcal{H} =< \omega \mid \mathcal{G} >$), we obtain from (1.13) and (1.15)

$$\begin{aligned} \mid \omega > \; &= \; \sum_{n=0}^{\infty} \frac{1}{n!} \mid v >^{(n)} = \sum_{n=0}^{\infty} \frac{1}{n!} \, A^n \mid v >^{(0)} \\ &= \; T \, (\sum_{n=0}^{\infty} \frac{1}{n!} \, A_d^n) \, T^{-1} \mid v >^{(0)} \end{aligned} \qquad (1.16)$$

and therefore

$$\omega_i = \sum_{k,l=1}^{p} \, e^{\lambda_k} \, T_{ik} T_{kl}^{-1} \, v_l^{(0)} \qquad (1.17)$$

The m nonlinear coupled equations $\{\nu_\alpha(\{\phi_\beta\}) = 0; \; \alpha, \beta = 1, \ldots, m\}$ give the required solutions $\tilde{\phi}_\alpha$ and at the end we are left with

$$\mathcal{H}_D = \sum_{i=1}^{l} \tilde{\gamma}_i \, h_i, \quad \tilde{\gamma}_i = \gamma_i(\{\tilde{\phi}_\alpha\}). \qquad (1.18)$$

1.4 The order parameters

Let us now show how it is possible to associate the appearance of order parameters with the dynamical group, as well as the symmetry group, of the system in question, in the case of abelian broken symmetries [14].

The mean-field approximation to the system, represented by the hamiltonian H_{MF}, in the ordered state has a reduced hamiltonian H_{red}, that is an element of (a representation of) the SGA of the system. The hamiltonian H of the system, in the

disordered phase is not, in general, an element of this SGA; however, there may be an element of the SGA, let us call it H_{sym}, that effectively recovers the symmetry of the original hamiltonian H. When this happens, then, as far as symmetry is concerned, one can use the $H_{sym} \rightarrow H_{red}$ transition to mimic the $H \rightarrow H_{red}$ phase transition; by means of the former, we can define the order parameters associated with the latter.

We shall assume that the reduced hamiltonian is a representation of an element x_{red} of a semisimple complex Lie algebra g. We shall identify the algebra g_s of the (abelian) symmetry group G with a subalgebra of the Cartan subalgebra h of g. Similarly, g_0 is the algebra of the subgroup G_0. We thus have

$$g_0 \subset g_s \subset h \subset g , \quad [H_{red}, g_0] = 0 , \quad \text{and} \quad [H_{red}, g_s] \neq 0 . \tag{1.19}$$

If H_{red} is diagonalizable, x_{red} belongs to some Cartan subalgebra $\bar{h}$ of g. Since, in the semisimple complex case, all Cartan subalgebras are conjugate under the adjoint group of g, we have an automorphism $\mathcal{I} : g \rightarrow g$, such that $h = \mathcal{I}(\bar{h})$. This automorphism enables us to define a new element $x_{sym} \in g$, by

$$x_{sym} = \mathcal{I}(x_{red}) \in h . \tag{1.20}$$

Since $[x_{sym} , g_s] = 0$, the Hilbert space representative H_{sym} of x_{sym} has the full symmetry of the original hamiltonian H and the same spectrum as H_{red}. Therefore we may label eigenstates of H_{sym} with symmetry labels appropriate to H; these are the eigenstates we use to mimic those of H and for which we require the order parameters to vanish. For example, the eigenstates of $\mathcal{H}_D$ in (1.18) are labelled by the eigenvalues λ_j of the h_j:

$$h_j| \{\lambda_j\} >= \lambda_j| \{\lambda_j\} > . \tag{1.21}$$

Let us define the order parameter η_A as the expectation value of an order operator $\mathcal{O}_A$ such that $\eta_A^d = 0$ in the disordered state $| d >$ but $\eta_A^g \neq 0$ in the ordered or broken symmetry ground state $| g >$. The state $| d >$ will be identified with a state in which the l mutually commuting operators $h_1, \ldots, h_l$ are all diagonal and represent then conserved quantities.

Now we see that the operators in Hilbert space corresponding to the non-Cartan elements e_α of the SGA behave as order operators. This follows from

$$< d | e_\alpha| d >= \frac{1}{\alpha_i} < d | [h_i, e_\alpha] | d >= 0 \tag{1.22}$$

provided that $\alpha_i \neq 0$. In that case, e_α will be an order parameter for the phase described by the non-conservation of the h_i, which form the subset $\bar{h}$ of $\{h_1, \ldots, h_l\}$. For a system with SGA of rank $l \geq 2$, the $e_\alpha, e_\beta, \ldots$ can correspond physically to coexisting order operators with order parameters $\eta_A^g, \eta_B^g, \ldots$, and a phase boundary can be defined in the space of coupling parameters $\{\beta_j, \mu_\alpha\}$ in H_{MF} by $\eta_A^g = \eta_B^g$, etc.

This approach manifestly fails in the case of non-Abelian broken symmetries such as, for example, the $SO(3)$ case of ferromagnetism. Here a typical model, $H = \sum_{i,j} J_{ij} S_i S_j$, which is $SO(3)$ invariant, leads to a mean-field reduction, $H_{red} = \sum_i \mu_i S_i$, which is not. However, the best one can do in this case, by an automorphism of the $so(3)$ SGA, to send H_{red} to $|\mu| S_3$ which does not recover the full $SO(3)$ symmetry. In chapter 2, we will present a scheme also including non-Abelian broken symmetries.

1.5   The conventional linearized BCS-model

The simplest model which illustrates the SGA method is the celebrated reduced BCS-model for the superconductivity [8]. The latter is recovered retaining, among the interaction terms in the hamiltonian (1.1), only the following term:

$$\frac{1}{2} \sum_{i,j} < i, -i \mid V \mid j, -j > a_i^\dagger a_{-i}^\dagger a_{-j} a_j, \qquad (1.23)$$

which correspond to the Cooper-pairing terms responsible for the superconductivity. Notice that the hamiltonian is invariant under the gauge transformation $a_k \rightarrow \exp(i\phi) a_k$ corresponding to the symmetry group $U(1)$.

Upon selecting $A \ (= B^\dagger)$ equal to $a_i^\dagger a_{-i}^\dagger$ in (1.3), and introducing the order parameter

$$\Delta_k := \frac{1}{2} \sum_j < k, -k \mid V \mid j, -j > < a_j a_{-j} >, \qquad (1.24)$$

the Hamiltonian H reduces to $H^{(1)}$, a direct sum of commuting single-k hamiltonians, i.e. $H^{(1)} = \sum_k H_k$,

$$H_k = \varepsilon_k (n_k + n_{-k}) + \Delta_k (a_k^\dagger a_{-k}^\dagger + a_{-k} a_k). \qquad (1.25)$$

H_k is readily seen to be an element of the Lie algebra $\mathcal{L} = su(2)$ generated by

$$J_+ = a_k^\dagger a_{-k}^\dagger = J_-^\dagger, \qquad J_3 = \frac{1}{2}(n_k + n_{-k} - 1). \qquad (1.26)$$

and therefore $H^{(1)}$ is an element of the SGA $g = \oplus_k su(2)_k$. In the basis (1.26), we have

$$H_k = 2\varepsilon_k J_3 + \Delta_k \ (J_+ + J_-) \tag{1.27}$$

and the diagonalization of H_k is then achieved through a Bogoliubov rotation $U = \exp \phi(J_+ - J_-)$ in the associated group space so that

$$H_k^{(d)} = U \ H_k \ U^{-1} = 2E_k J_3 \tag{1.28}$$

where $\phi = \frac{1}{2} \tan^{-1}(\Delta_k/\varepsilon_k)$ and $E_k = \sqrt{|\varepsilon_k|^2 + |\Delta_k|^2}$.

The eigenkets of $H_k^{(d)}$ are $su(2)$ states $| \ \Psi >$ which are labelled by the eigenvalues of J_3 and J^2, the Casimir operator of $su(2)$, for each k. Using the notation $| \ \Psi >= | \ J^2 J_3 >$, we have

$$H_k^{(d)} | \ \Psi > \ = \ 2E_k J_3 | \ J^2 J_3 >= 2E_k m | \ J^2 J_3 > \tag{1.29}$$

$$J^2 | \ J^2 J_3 > \ = \ j(j+1) | \ J^2 J_3 > . \tag{1.30}$$

From $J^2 = n_k n_{-k} + J_3 + J_3^2$, we deduce that both the Casimir and J_3 are functions only of the number operators $n_{\pm k}$ and that the only possibilities are therefore

$$J_3 \ \rightarrow \ m = \pm \frac{1}{2} \ \text{or} \ 0 \ , \tag{1.31}$$

$$J^2 \ \rightarrow \ j(j+1) = \frac{3}{4} \ \text{or} \ 0 \ . \tag{1.32}$$

Recalling that j also labels irreducible representation D^j of $su(2)$, the possible kets are

$$| \ J^2 J_3 >= \begin{cases} | \ \pm \frac{1}{2}, \frac{3}{4} >\sim D^{1/2} \ , \\ | \ 0, 0 >\sim \ D^0 \end{cases} \tag{1.33}$$

The eigenket of H_k is then $| \ \Phi >= U^{-1} | \ J^2 J_3 >$ and the representation labels $j = 1/2, 0$ distinguish physically different states. States given by $U^{-1} | \pm 1/2, 3/4 >$ are excited $(+1/2)$ and ground $(-1/2)$ "pairs" while $U^{-1} | \ 0, 0 >$ states are "singles". The ground state has energy $-E_k/2$, in accord with the physical expectation that both constituents of the pair are occupied, i.e. $n_k = n_{-k} = 1$ and $m = -1/2$.

In fact, the identification of different types of states (excitations or quasi-particles) with irreducible representation of the SGA is a general feature in all these many body systems. Another important point that we do not treat here is the fact that the many fermion Green functions for $T = 0$ and $T \neq 0$ are built up from factors completely determined by the Dynamical Algebra.

1.6 Dynamical su(8) for phase-coexistence

Considerable interest, both theoretical and experimental has been aroused by evidence of the presence of coexisting phases in certain alloys at low temperatures. The main question investigated is the relation between the SGA of the coexisting phases and its subalgebras, and the connections with uncoupled phases.

Let us describe a multi-phase interacting system of electrons [15]. For this purpose, we introduce a mean-field hamiltonian which incorporates (apart from the usual kinetic energy term (H_{ke})), singlet superconductivity (H_{sc}), charge-density (H_{cdw}) and spin-density wave (H_{sdw}) terms. Thus

$$H = H_{ke} + H_{sc} + H_{cdw} + H_{sdw} \tag{1.34}$$

where

$$H_{ke} = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} \tag{1.35}$$

$$H_{sc} = \sum_k \Delta^*_k a_{k\uparrow} a_{-k\downarrow} + \text{h.c.} \tag{1.36}$$

$$H_{cdw} = \sum_{k,\sigma} \gamma^0_k \, a^\dagger_{k+Q,\sigma} a_{k\sigma} + \text{h.c.} \tag{1.37}$$

$$H_{sdw} = \sum_k a^\dagger_{k+Q} \, \underline{\gamma} \cdot \underline{\sigma} \, a_{k\sigma} + \text{h.c.} \tag{1.38}$$

Charge-density waves (CDW) are associated to periodic lattice distortions occuring at low temperatures for certain quasi-one-dimensional crystalline compounds. The conduction electrons will attempt to screen the periodic potential set up by the atomic displacements, and the CDW describes the density modulation of the electrons near the Fermi surface. Since the compounds showing this phase transition (referred to as Peierls transition) may also be superconducting, there is the possibility to observe the simultaneous occurence of both states, SC and CDW, in a given sample.

Above, $Q = 2k_F$ is a characteristic wave vector for density wave order. With the additional semplification that there is no contribution from terms for which $|k| > Q$, we may write $H = \oplus_k^{k_F} H(k)$, where $H(k)$ is a bilinear in the set

$$\{A_i(k)\} = \{\, a_{k\uparrow} \, , \, a^\dagger_{-k\downarrow} \, , \, a_{\bar{k}\uparrow} \, , \, a^\dagger_{-\bar{k}\downarrow} \, ; \, a_{k\downarrow} \, , \, a^\dagger_{-k\uparrow} \, , \, a_{\bar{k}\downarrow} \, , \, a^\dagger_{-\bar{k}\uparrow} \,\} \quad , \tag{1.39}$$

where $\bar{k} = k - Q$. It is then easy to verify that $\{A_i(k) \, , \, A_j(k')\} = \delta_{ij}\delta_{kk'}$ and that $X^i_j = A^\dagger_i A_j$ $(i,j = 1,\ldots,8)$ generate the Lie algebra $gl(8)$. The hamiltonian, due

to its hermiticity, may be considered as an element of $su(8)$ and the SGA is thus $\oplus_k su(8)_k$.

The Lie algebra $su(8)$ is an algebra of order 63 and rank 7. Following the discussion in section(1.4), we try to classify the order parameters for the model. We have the seven commuting Cartan elements h_i, corresponding to operators such as number, spin, momentum, etc., which are no longer conserved in the transition to broken symmetry phase and 56 order parameters corresponding to the elements e_α. These order operators consist of four quartets (singlet plus triplet, of differing parity and time-reversal sign) for each of the superconductivity type $a_k a_{-k}$, density wave $a_k^\dagger a_{k-Q}$ and anomalous type $a_k a_{-(k-Q)}$ operators, together with 8 ferromagnetic operators.

From this system of operators, we may derive various chains of subalgebras, considering the centralizers $C(h_i)$ of the relevant h_i, and their complement $\bar{C}(h_i)$. For example, density wave terms conserve the electron number

$$\hat{N} = \sum_k N_k \quad , \quad N_k = \sum_{\sigma=\uparrow\downarrow} (n_{k\sigma} + n_{-k\sigma} + n_{\bar{k}\sigma} + n_{-\bar{k}\sigma}) \tag{1.40}$$

while superconducting (and anomalous) type do not. Therefore

$$g_{dw} = C_{su(8)}(N_k) = u(1) \oplus su(4) \oplus su(4) \quad . \tag{1.41}$$

The pure CDW-phase SGA is given by the centralizer of the spin operator

$$\underline{\sigma}(k) = \sum_{p=\pm k, \pm \bar{k}} \sum_{\alpha,\beta} a_{p\alpha}^\dagger \underline{\sigma}^{\alpha\beta} a_{p\beta} \quad , \tag{1.42}$$

since the CDW waves conserve spin; thus

$$g_{cdw} = C_{g_{dw}}(\underline{\sigma}(k)) = u(1) \oplus so(4) \quad . \tag{1.43}$$

In this case, we expect four $\hat{N}$-invariant order-parameters corresponding to breaking of momentum P and the $k, \bar{k}$-number difference $S = (N_k - N_{\bar{k}})/2$, these being the operators corresponding to the two Cartan of $so(4)$. There are four root vectors and therefore four independent order parameters. They may be most simply obtained from the operator

$$X_3^1 + X_7^5 = a_{k\uparrow}^\dagger a_{\bar{k}\uparrow} + a_{k\downarrow}^\dagger a_{\bar{k}\downarrow} \tag{1.44}$$

by parity π transformation [3] and hermitian conjugation. For real coupling constant γ_0, the SGA reduces to $u(2) \sim u(1) \oplus so(3)$.

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[3]The parity transformation is defined in the following way: $\pi a_{k\sigma}\pi^\dagger = a_{-k\sigma}$, $\pi a_{\bar{k}\sigma}\pi^\dagger = a_{-\bar{k}\sigma}$.
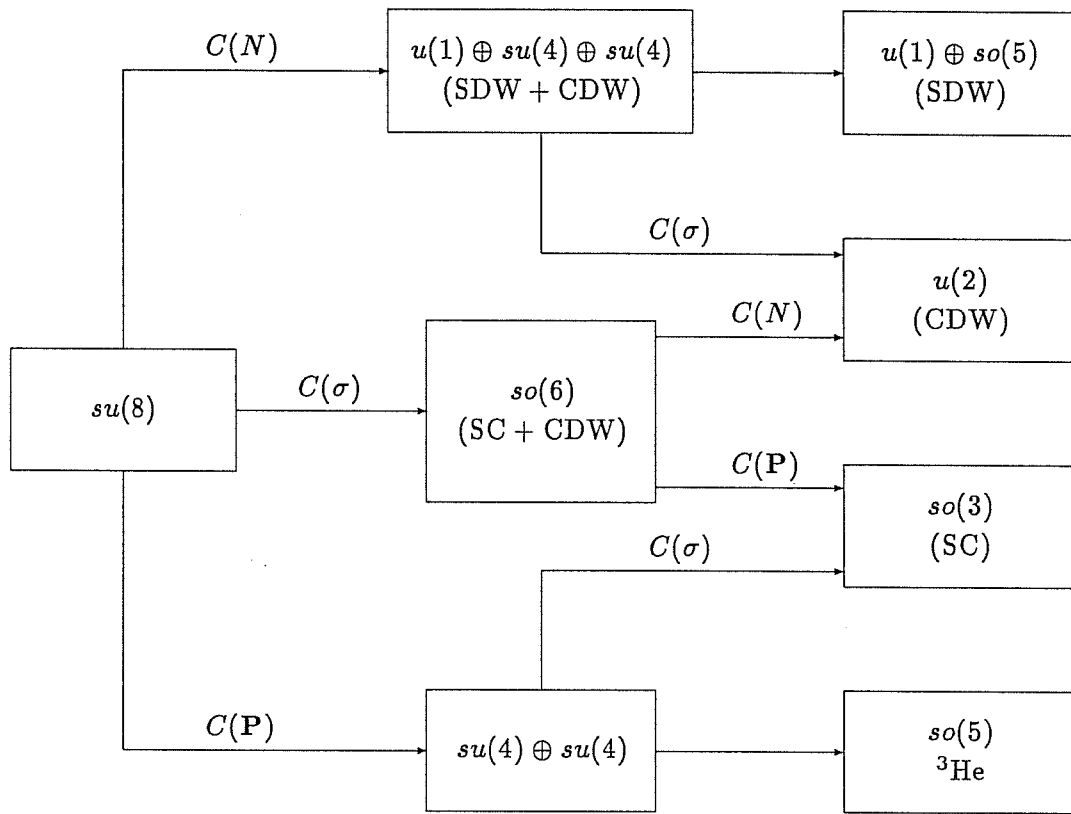
Figure 1.1: SGA cascade from $su(8)$

The SDW wave case correspond to $\gamma_0 = 0$; this has SGA

$$g_{sdw} = u(1) \oplus so(5) \oplus so(5) \quad . \tag{1.45}$$

The center $u(1)$ is again generated by the total number operator N; the four other Cartan of $so(5) \oplus so(5)$ correspond to P, S, σ_3, and $\underline{P} \cdot \underline{\sigma}$ number S'. There are sixteen root vectors, and therefore potentially sixteen order parameters. However, four of these commute with P, and so there are only twelve SDW order parameters, which split into 4 spin triplets. Again, these may most simply be generated from the operator

$$X_3^1 - X_7^5 = a_{k\uparrow}^\dagger a_{\bar{k}\uparrow} - a_{k\downarrow}^\dagger a_{\bar{k}\downarrow} \tag{1.46}$$

by spin-rotation $\underline{\sigma}$, parity π and hermitian conjugation. For real coupling constants $\underline{\gamma}$, the SGA reduces to $u(1) \oplus so(5)$.

In figure (1.1), we illustrate the subgroup descent from $su(8)$ which encompass the phenomena described so far.

We have seen that the above algebras are all reductive, with the $u(1)$ component being generated by the number operator (1.40) as central element. If in addition, the so-called "nesting" condition is imposed, $\varepsilon(k) + \varepsilon(\bar{k}) = 0$, then the SGA's will reduce to their semi-simple component.

1.7 The supersymmetric linearized BCS-model

If we use Fermi-linearization instead of the usual bosonic linearization method, we are led to SGA which are superalgebras. Lie superalgebras are $\mathbb{Z}_2$-graded vector spaces with a bosonic (even) $\mathcal{B}$ sector and a fermionic (odd) $\mathcal{F}$ sector. [4] An hamiltonian $\mathcal{H}$ is said to be supersymmetric if it exists a charge operator $Q \in \mathcal{F}$ such that

$$\mathcal{H} = \{Q, Q^\dagger\} \quad , \quad Q^2 = Q^{\dagger^2} = 0 \quad . \tag{1.47}$$

In this section, we show how the BCS model may be regarded as the hamiltonian of a model exhibiting spontaneously broken supersymmetry [53].

First, we consider, together with (1.23), interactions of umklapp type ([62]) retaining terms of the type

$$\frac{1}{2} \sum_{i,j} < i,j \mid V \mid -j, -i > a_i^\dagger a_j^\dagger a_{-i} a_{-j}, \qquad 2\,(\mathbf{i}+\mathbf{j}) \in \Lambda^\# \tag{1.48}$$

---

[4] For more details about superalgebras and supersymmetry, see appendix B

where $\Lambda^{\#}$ is the reciprocal lattice of the crystal and define the new order parameter

$$\delta_k := \frac{1}{2}\sum_j < k, j \mid V \mid - j, -k >< a_j^{\dagger} a_j > \quad . \tag{1.49}$$

Then H_k in equation (1.25) modifies to

$$\mathcal{H}_k = \varepsilon_k(n_k + n_{-k}) + (\Delta_k a_k^{\dagger} a_{-k}^{\dagger} + \delta_k a_k^{\dagger} a_{-k} + \text{h.c.}). \tag{1.50}$$

which belongs to the Lie algebra $su(2) \oplus su(2)$.

Now let us retain other terms from the general hamiltonian (1.1) coming from the following umklapp (momentum non-conserving) processes:

$$\frac{1}{2}\sum_{i,j} < i, -i|V|j, i > a_i^{\dagger} a_{-i}^{\dagger} a_i a_j, \qquad (\mathbf{i}+\mathbf{j}) \in \Lambda^{\#} \tag{1.51}$$

$$\frac{1}{2}\sum_{i,j} < i, -i|V|j, -i > a_i^{\dagger} a_{-i}^{\dagger} a_{-i} a_j, \quad (\mathbf{i}-\mathbf{j}) \in \Lambda^{\#} \tag{1.52}$$

We then Fermi-linearize these terms as shown in subsection (1.2.2). The new resulting linearized hamiltonian $H_k^{(S)}$ is recognized to be an element of the Lie superalgebra $su(2|2)$ where the bosonic sector $\mathcal{B}$ is the $su(2) \oplus su(2)$ Lie algebra $\mathcal{L}$ of $\mathcal{H}_k$

$$\left\{ a_+^{\dagger} a_-^{\dagger} \ , \ a_- a_+ \ , \ \frac{1}{2}(n_+ + n_- - 1) \right\} \oplus \left\{ a_+^{\dagger} a_- \ , \ a_-^{\dagger} a_+ \ , \ \frac{1}{2}(n_+ - n_-) \right\} \quad , \tag{1.53}$$

and the fermionic sector $\mathcal{F}$ is given by the eight operators

$$\left\{ a_{\pm}(1 - n_{\mp}) \, , \ a_{\pm}^{\dagger}(1 - n_{\mp}) \, , \ n_{\pm} a_{\mp} \, , \ a_{\pm}^{\dagger} n_{\mp} \right\} \quad . \tag{1.54}$$

Here and in the following, we omit the subindex k setting $a_{\pm} \equiv a_{\pm k}$. Therefore, we can write $H_k^{(S)} = \mathcal{H}_k + H_k^{(F)}$, where

$$H_k^{(F)} = \sum_{F_i \in \mathcal{F}} v_i \, F_i \quad , \quad v_i \in \mathcal{G} \quad . \tag{1.55}$$

Let us now show how $\mathcal{H}_k$ can be considered as a supersymmetric hamiltonian in terms of charge operators $Q, Q^{\dagger} \in \mathcal{F}(su(2|2))$. We define

$$\tilde{\mathcal{H}}_k = \varepsilon_k n_+ + \varepsilon_- n_- + (\Delta_k a_+^{\dagger} a_-^{\dagger} + \delta_k a_+^{\dagger} a_- + \text{h.c.}) \tag{1.56}$$

which is a generic element of $su(2) \oplus su(2)$ and the charge Q:

$$Q = \alpha a_+ n_- + \beta a_- n_+ + \gamma a_+^{\dagger}(1 - n_-) + \delta a_-^{\dagger}(1 - n_+) \tag{1.57}$$

$E_k^{(1)}$

$c - e_+$

$$|f> = \frac{1}{\sqrt{2}}(|10> + |01>) \qquad |b> = \frac{1}{\sqrt{2|\delta_k|}}(e_+^{1/2}|00> + e_-^{1/2}|11>)$$

$(F) \qquad \xleftarrow{\qquad Q \, , \, Q^\dagger \qquad} \qquad (B)$

$$|f_0> = \frac{1}{\sqrt{2}}(|10> - |01>) \qquad |b_0> = \frac{1}{\sqrt{2|\delta_k|}}(e_+^{1/2}|00> - e_-^{1/2}|11>)$$

$c - e_-$
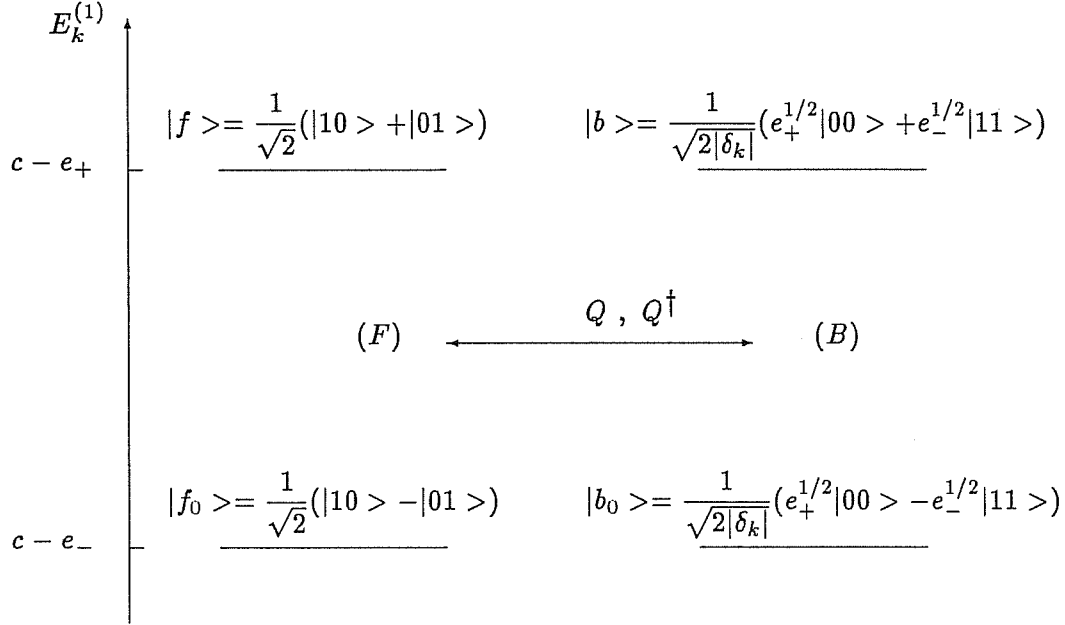
Figure 1.2: The energy spectrum of $\tilde{\mathcal{H}}_k$

which is an element of $\mathcal{F}(su(2|2))$ and whose square is zero. Then provided $|\alpha|^2 - |\gamma|^2 = \varepsilon_-$, $|\beta|^2 - |\delta|^2 = \varepsilon_+$, $\beta^*\gamma - \alpha^*\delta = \Delta_k$ and $\delta^*\gamma - \alpha^*\beta = \delta_k$, we may express the hamiltonian (1.56), up to an additive constant $c = |\gamma|^2 + |\delta|^2$, as

$$\tilde{\mathcal{H}}_k = \{Q, Q^\dagger\} \quad , \text{with} \quad [\tilde{\mathcal{H}}_k, Q] = 0. \tag{1.58}$$

In this case the potentials must satisfy $|\delta_k|^2 = |\Delta_k| + \varepsilon_+\varepsilon_-$ and we have a spontaneously broken supersymmetric model; $\tilde{\mathcal{H}}_k$ satisfies (1.58) but $Q^\dagger|f_0> \neq 0$ and $Q|b_0> \neq 0$ (unless $c = |\delta_k| - (\varepsilon_+\varepsilon_-)^{\frac{1}{2}}$), where $\{|f_0>, |b_0>\}$ is the degenerate ground state of the model. In figure (1.2), we exhibit the spectrum of this system in the basis $\{|n_+ \; n_->\}$, where $c = |\gamma|^2 + |\delta|^2$ and $e_\pm = |\delta|_k \pm (\varepsilon_+\varepsilon_-)^{1/2}$.

But if the pairing order parameter Δ_k vanishes ($\gamma = \delta = 0$), then we obtain an Hamiltonian

$$\mathcal{H}_k^{(0)} = \varepsilon_+ n_- + \varepsilon_- n_+ + \delta_k a_+^\dagger a_- + \delta_k^* a_-^\dagger a_+ \quad . \tag{1.59}$$
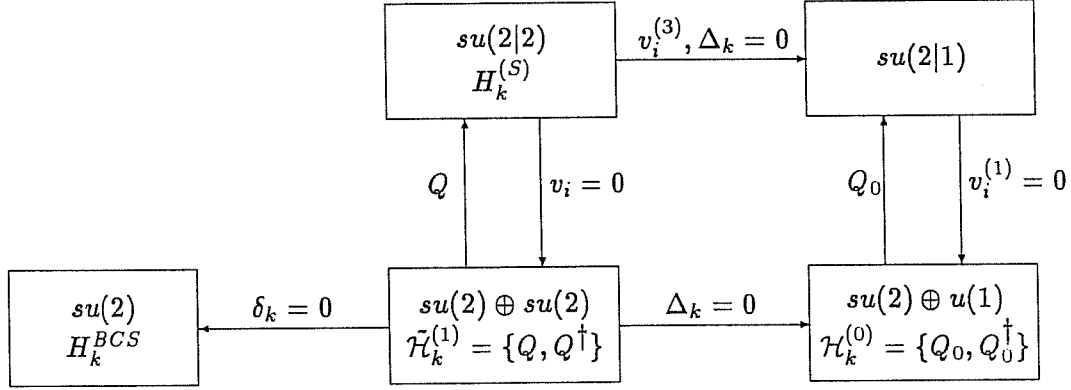
Figure 1.3: Lie algebra-superalgebra chain

with $\delta_k = \exp(i\phi_k)(\varepsilon_+\varepsilon_-)^{\frac{1}{2}}$. The hamiltonian $\mathcal{H}_k^{(0)}$ describes a system with unbroken supersymmetry, because $\mathcal{H}_k^{(0)} = \{Q_0, Q_0^\dagger\}$ with

$$Q_0 = \sqrt{\varepsilon_-}\; a_+ n_- - e^{-i\phi_k}\sqrt{\varepsilon_+}\; a_- n_+, \quad Q_0^2 = 0, \tag{1.60}$$

such that $[\;\mathcal{H}_k^{(0)}, Q_0\;] = 0$ and $Q_0, Q_0^\dagger$ annihilate the (degenerate) ground state $\{\frac{1}{\sqrt{2}}(|1,0> -|0,1>),\; |0,0>\}$.

Identifying Δ_k as the superconducting order parameter, $\mathcal{H}^{(0)}$ describes a system above the critical temperature for pairing, where $\Delta_k = 0$ and $|\delta_k| \neq 0$. In this sense, the superconductive phase transition may be considered as a spontaneous breaking of supersymmetry for this model.

Notice that the SGA of $\mathcal{H}_k^{(0)}$ is the algebra $u(2)$ generated by

$$\left\{\frac{1}{2}(n_+ + n_- - 1)\;,\; \frac{1}{2}(n_+ - n_-)\;,\; a_+^\dagger a_-\;,\; a_-^\dagger a_+\right\} \quad . \tag{1.61}$$

The appropriate superalgebra for the discussion of this model is that obtained adding the fermionic elements $\{a_\pm n_\mp\;,\; a_\mp^\dagger n_\pm\}$ of Q_0 and $Q_0^\dagger$. The resulting superalgebra is $su(2|1)$.

In figure(1.3) we give a diagram of the connections between the various Lie algebras and superalgebras of the models discussed above. The coefficients $v_i^{(1)}$ are related to terms of the type $< a_i >$, $v_i^{(3)}$ to terms of the type $< a_i a_j a_k >$.

Chapter 2

Fermi-linearization on Hubbard-like models

2.1 Transition metals and compounds.

An interesting group of solids is the family of materials containing transition-group elements whose atoms have incomplete d or f subshells.

Metals and alloys in which atomic magnetic ordering (ferro-, antiferro- or ferrimagnetic) is observed in a certain temperature interval requires that at least one of the constituents be a transition element. In these materials, many-electrons effects are manifest very intensively and even when they possess no magnetic order, they still exhibit unusual thermal, magnetic, optical, electrical and even mechanical properties. The nature of these anomalies is due to the peculiar behavior of d and f states.

Let us consider the atom of a transition element. First we have to pay attention to the small radius of d electron and particularly f electron subshells in comparision with characteristic distance between nearest ions in the metallic state of a relevant element. Another interesting feature is that the filling of d and f subshells proceeds in jumps at the middle and end of each series. This indicates that the one-electron approach is inadequate to describe the atoms of the transition elements and we have to take account of the exchange correlation interaction, which leads to the formation of an atomic magnetic moment.

When atoms are united into a crystal, the electronic states which we are concerned primarily with are the states of unfilled shells, for these states are responsible for almost all the properties of the crystal. When atomic states form a band we

have a gain in kinetic energy and a loss in Coulomb repulsive energy. If the radius of a relevant electron subshell exceeds the nearest atom or ion distance, Bloch states arise. This situation occurs for outer s - and p -shell electrons, giving rise to metals, covalent bonds or ionic crystals.

A different situation occurs in rare-earth metals for the states of f electrons, which are believed to be well localized (~ 0.3 Å). These electrons maintain their atomlike character and do not form a band, so that their magnetic moment in compounds or in the metallic state are normally close to those of the corresponding atoms.

Both cases may be realized for d states. The atomlike behavior of d -states persists in many semiconducting compounds (f.ex. NiO). In other cases metal-insulator transitions occur. But despite the efforts during the last decades, the problem of constructing a unified description of the "localized itinerant" behavior of d-electrons is still far from being resolved, even if on the whole the problem as to the nature of d states is solved rather in favor of their band character.

The simplest models describing such systems are characterized by a kinetic term describing the motion of the electrons and a local electron-electron coupling and are generally called Hubbard-like models. The class of these models can be described by a general second quantized Hamiltonian

$$H = \sum_{\sigma} \sum_{\alpha\alpha'} \sum_{ij} t^{\alpha\alpha'}_{\sigma,ij} \, a^{\dagger}_{\alpha\sigma,i} a_{\alpha'\sigma,j} + \sum_{\alpha,i} U_{\alpha} n_{\alpha\sigma,i} n_{\alpha,-\sigma,i} \tag{2.1}$$

where σ, α are spin and band indices respectively, U_{α} and $t^{\alpha\alpha'}_{\sigma,ij}$ are the Coulomb strenght and the hopping amplitude.

2.2   The Hubbard model and high-T_C superconductivity

The Hubbard hamiltonian is the simplest model describing strongly correlated electrons. It appeared in the literature for the first time in 1963, in two subsequent independent papers of Gutzwiller and Hubbard [40], and is characterized by a nearest-neighbour hopping. In its one-band version, it reads

$$H = - \sum_{<i,j>} \sum_{\sigma} t_{ij}(a^{\dagger}_{i\sigma} a_{j,\sigma} + a^{\dagger}_{j\sigma} a_{i,\sigma}) + \sum_{i\in\Lambda} U_i n_{i\uparrow} n_{i\downarrow} \quad , \tag{2.2}$$

where the sums run over the lattice sites, the symbol $< i,j >$ indicates a sum over nearest-neighbor pairs and t_{ij} is the hopping integral. $U > 0$ corresponds to

repulsive Coulomb interaction, whereas $U < 0$ could eventually describe an effective attractive interaction mediated by ions.

The hamiltonian (2.2) is commonly agreed to be the ideal tool to describe the relevant collective features of the transition metals, namely itinerant magnetism and metal-insulator (or Mott) transition. Indeed, for $U = 0$, H reduces to a system of non-interacting moving electrons, while in the atomic limit ($t = 0$), the electrons are fully localized and at half- filling, the system is insulating. The latter feature still holds for finite t and $U = \infty$, and the corresponding system has been shown to be an antiferromagnetic insulator.

For intermediate couplings, the model is exactly solvable only in one dimension, where Mott transition is absent at any $T \neq 0$, according to the Mermin-Wagner theorem. The failure of the attempts in finding exact statistical mechanics solutions in dimension greater than one has stimulated the growth of several approximate methods. For example, in the so-called strong coupling limit characterized by $|t| <<$ U, which is the most appropriate physical region in dealing with strongly correlated electron systems, the Mott transition and the magnetic behaviour of the model have received partial answer. The main result is that to second-order in $|t|/U$ and at exact half-filling, the Hubbard hamiltonian can be mapped into an antiferromagnetic Heisenberg hamiltonian

$$H = \sum_{<i,j>} J_{ij} \{ \mathbf{S}_i \mathbf{S}_j - \frac{1}{4} \} \quad , \quad J_{ij} > 0 \tag{2.3}$$

where

$$J_{ij} = 4 \frac{|t_{ij}|^2}{U} \quad , \quad \mathbf{S}_i = \frac{1}{2} \sum_{\mu\mu'} a_{i\mu}^\dagger [\sigma]_{\mu\mu'} a_{i\mu'} \quad , \tag{2.4}$$

thus exhibiting clearly the dominant role of the magnetic correlations in limit of strong Coulomb repulsion.

Since the discovery of superconducting materials with unexpectedly high transition temperatures, a large variety of mechanisms and new concepts (spin liquids [4], spin and charge bags [68], anyons [27], etc.) have been proposed but the origin of this phenomenon however is still unclear. Namely these transition temperatures exceed the upper limits which can be deduced on the basis of the present understanding of the BCS-mechanism, that is retarded electron-electron attraction via phonons.

The main theoretical efforts has been devoted to model the CuO systems, which are believed to contain the relevant physics of the new superconducting materials. Typically, they are ceramic layered compounds with a highly complex unit cell, which becomes superconducting upon doping, an example being $La_{2-x} (X)_x Cu O_4$ with

X=Ba, Sr. Their behaviour falls into two distinct regimes, depending on doping. Pure samples are considered to be good examples of Mott insulators. At low doping, they are bad metals and exhibit the Mott transition with magnetism characteristic of transition metal oxides, phenomena originating in the strong intraatomic Coulomb interaction between poorly screened electrons. At high doping, they become high-T_c superconductors and are quite good metals, with the antiferromagnetic phase being remarkably close to the superconducting one.

Therefore, the interplay between magnetic behavior and Mott transition near half-filling (from stochiometric measurements) seems to play a crucial role, and this has led theorists to seriously reconsider the physical properties of the Hubbard model and its extensions. Especially the two-dimensional strong-coupling version of the model (the so-called $t - J$ model) has been extensively investigated.

However, for the Hubbard model itself, numerical studies are restricted to small lattices and it thus seems unclear, up to now, whether models of strongly correlated fermions could have a superconductive ground state.

We conclude this section mentioning the anyon superconductivity. This scenario suggested by Laughlin ([46]) is based on the idea that in three space-time dimensions, one has the possibility of particle excitations with non-integer statistics, called anyons. The mechanism leading to superconductivity can be summarized as follows: anyons in a planar sample attract each other with a vector (gauge) interaction that is necessarily present in anyon theories. If the excitations are also electrically charged such attraction can be made strong enough so as to overcome Coulomb repulsion and bind the excitations in pairs (as Cooper pairs in conventional BCS theories), producing superconductivity. A review about the interrelations between the Hubbard model and anyon superconductivity can be found in [7].

2.3   The Yang-Zhang SO(4) symmetry

Let us rewrite the Hubbard model (2.2) in the grand-canonical ensemble:

$$H = -\mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) - t \sum_{<i,j>} \sum_\sigma a^\dagger_{i,\sigma} a_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad , \tag{2.5}$$

where μ is the chemical potential.

In a recent paper [79], C.N. Yang and S.C. Zhang have shown that the model at half filling is endowed with a global $SO_4 = (SU_2 \otimes SU_2)/\mathbb{Z}_2$ symmetry.

At half filling ($\mu = \frac{1}{2}U$) one can indeed check that hamiltonian (2.5) as well as the total momentum operator commute with two mutually orthogonal $su(2)$ algebras.

The first *spin su(2)* is generated by the operators

$$S_+ = \sum_i a_{i\uparrow}^\dagger a_{i\downarrow} \equiv \sum_k a_{k\uparrow}^\dagger a_{k\downarrow} \quad , \quad S_- = S_+^\dagger$$

$$S_0 = \frac{1}{2}\sum_i (n_{i\uparrow} - n_{i\downarrow}) \equiv \frac{1}{2}\sum_k (n_{k\uparrow} - n_{k\downarrow}) \quad , \tag{2.6}$$

with the usual $su(2)$ algebra $[S_0, S_\pm] = \pm S_\pm$, $[S_+, S_-] = 2S_0$, and derives from the fact that the interaction is isotropic in spin space. However, besides this "obvious" symmetry, there is a "hidden" *pseudospin su(2)* symmetry, which is generated by

$$J_+ = \sum_j e^{i\mathbf{p}\cdot\mathbf{j}} a_{j\downarrow}^\dagger a_{j\uparrow}^\dagger \equiv \sum_k a_{k\uparrow}^\dagger a_{p-k\downarrow}^\dagger \quad , \quad J_- = J_+^\dagger$$

$$J_0 = \frac{1}{2}\sum_i (n_{i\uparrow} + n_{i\downarrow} - 1) \equiv \frac{1}{2}\sum_k (n_{k\uparrow} + n_{k\downarrow} - 1) \quad , \tag{2.7}$$

where $\mathbf{p}$ is the vector (π, π, π). By $a_{k\sigma}$, we denote the Fourier transforms of $a_{i\sigma}$.

When the condition of half filling is not met, J_0 still commutes with the hamiltonian, due to the conservation of the particle number but J_+ and J_- do not, and the global symmetry of the model is $u(1) \oplus su(2)$ generated by $\{J_0; S_+, S_-, S_0\}$.

The physical meaning of (2.7) can be understood as a coherent resonant excitation of the system. This remarkable fact is due to the particular combination of both the kinetic and the potential energies in (2.5).

The $\mathbb{Z}_2$ present in the full global symmetry is a duality transformation given by a unitary operator $\hat{U}$ such that

$$\hat{U} a_{i\uparrow}\hat{U}^{-1} = a_{i\uparrow}^\dagger \quad , \quad \hat{U} a_{i\downarrow}\hat{U}^{-1} = (-1)^i a_{i\downarrow}^\dagger \quad , \tag{2.8}$$

which exactly interchanges the spin with the pseudospin algebra. This transformation is known to transform the negative U Hubbard model in the positive U model.

It is crucial to observe that $J^2 = \frac{1}{2}\{J_+, J_-\} + J_0^2$ is an exact conserved quantity. Therefore, the four quantum number associated to S^2, S_0, J^2, J_0 can be used to classify all the eigenstates of the Hubbard model. An important consequence of this fact is the exact one-to-one correspondence of the states at half-filling ($\mu = U/2, J_0 = 0$) and the states away from half-filling.

In the superconducting phase, the $U(1)$ symmetry associated to J_0 is spontaneously broken. From a generalization of the Goldstone theorem, Zhang proved that, for the Hubbard model, if the ground state is superconducting, there must exist a triplet of collective excitations, with energies $\pm(U - 2\mu)$, 0. Experimental detection of these new modes could answer the question whether the Hubbard model describes the high-T_C superconductors.

2.4   Symmetry breaking and order parameters

In this section, we shall discuss how the different mean-field approaches to the Hubbard model may affect the Yang-Zhang symmetry, as well as the dynamical algebra emerging in the approximation scheme, and which relevant order parameters are generated by the related symmetry breaking processes [49].

In the sequel we shall denote by $g_s^{(n)}$ the algebra of the symmetry group of (1) corresponding to filling n (n is the average occupation number $n \doteq \dfrac{< N_e >}{N_\Lambda}$; N_e and N_Λ denoting, respectively, the total number of electrons operator and the number of sites). Half filling implies $n = 1$, and $g_s^{(1)} = su(2) \oplus su(2)$.

Let us denote by g_d the dynamical algebra of the linearized hamiltonian H_ℓ. Naturally, the process of linearization affects only part of the hamiltonian. We denote by $H^{(0)}$ the part of H not affected by the approximation. In other words, $H = H^{(0)} + H^{(I)}$, and $H_\ell = H^{(0)} + H_\ell^{(I)}$. $H^{(0)}$ and $H_\ell^{(I)}$ have themselves dynamical algebras which are subalgebras of g_d, and we denote them by $g_d^{(0)}$ and $g_d^{(I)}$ respectively.

In section (1.4), the order parameters associated with the breaking of abelian symmetries were defined as the expectations of those operators in g_d generating its root space. This identification holds when, besides being abelian, g_s is a subalgebra of the Cartan subalgebra h_d of g_d: the order parameters correspond to the breaking of the symmetries induced by the operators in $g_s \cap h_d$. A natural generalization of the above scheme, also holding for non-abelian symmetries, is the following[1] :

- construct the commutator set $g \doteq [H_\ell, g_d]$;

- define the set $g' \doteq g_d/g$;

- define $g_p = \begin{cases} g'/g_d^{(0)}, & \text{if } g_d = g_d^{(0)} \oplus g_d^{(I)}; \\ g' \setminus g_d^{(0)}, & \text{otherwise}; \end{cases}$

- identify the order parameters as the averages of the operators $\mathcal{P}_i \in g_p$.

This procedure implies that $< \mathcal{P}_i >$ is non identically vanishing, $< \bullet >$ denoting some average over H_ℓ (for instance, it can represent a statistical average over a Gibbs ensemble or the expectation value over the ground state). Any mean field strategy can now be made explicit by constructing suitable consistency equations for $< \mathcal{P}_i >$.

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[1]When the operation is not defined with algebras, we denote by the symbol / subtraction of the common generators in the basis fixed by g. On the other hand the symbol \ denotes subtraction element by element of common operators

In general, one should expect that in the disordered phase (corresponding to vanishing order parameters) the whole symmetry g_s were restored for the linearized model and in fact this happens for most of the bosonic and for the fermionic linearization schemes . However, this is not always the case and the phase described by the vanishing of the order parameter may still be an ordered phase.

2.4.1 Bosonic Linearization Schemes

Three different bosonic linearization schemes have been adopted for the Hubbard model, all of which approximate the on-site interaction U term, quadrilinear in the fermionic operators, by a combination of bilinear terms. Such schemes lead therefore to a description suitable for the weak coupling regime in which the electrons exhibit a band-like behavior (*i.e.* they are almost delocalized). The dynamical algebra for the resulting hamiltonian is easily recognizable in all cases if one represents the site-dependent operators in their Fourier transformed form. In particular, in the latter representation one immediately verifies that $g_d^{(0)} \equiv \bigoplus_k u(1)_k$, each $u(1)_k$ generated by

$$L_z^{(k)} \doteq \frac{1}{2}(n_{k\uparrow} + n_{k\downarrow} - 1) \quad , \tag{2.9}$$

as the tight-binding model is diagonal in wave-vector space.

The Hartree Approximation

In this case ([37]), the hamiltonian (2.5) is modified by assuming

$$n_{i\uparrow}n_{i\downarrow} \mapsto \left(\alpha - \frac{1}{2}\right)(n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2}\alpha^2 \quad , \tag{2.10}$$

where $\alpha = < n_{i\uparrow} + n_{i\downarrow} >$. The resulting linearized hamiltonian H'_ℓ reads

$$H'_\ell = \sum_k \left[\varepsilon_k + U\left(\alpha - \frac{1}{2}\right)\right](2L_z^{(k)} + 1) + \frac{1}{2}N_\Lambda U\alpha^2 \tag{2.11}$$

where $\varepsilon_k \doteq -\mu + 2t\sum_{r=1}^{d} \cos(k_r)$. H'_ℓ is manifestly diagonal in its wave-vector space representation, and its dynamical algebra g_d coincides with $g_d^{(0)}$. Since H'_ℓ is invariant with respect to all of the transformations generated by $g_s^{(n)}$, the linearization does not provide, any non-trivial order parameter.

The Hartree-Fock Approximation

This approximation ([75]) consists in substituting

$$n_{i\uparrow}n_{i\downarrow} \mapsto \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + \gamma a_{i\uparrow}a_{i\downarrow}^{\dagger} + \gamma^* a_{i\downarrow}a_{i\uparrow}^{\dagger} + |\gamma|^2 \quad ; \qquad (2.12)$$

where $\gamma = < a_{i\uparrow}^{\dagger}a_{i\downarrow} > \equiv |\gamma|e^{i\varphi_{\gamma}}$. The linearized hamiltonian H_{ℓ}'' has the form

$$H_{\ell}'' = \sum_k \left(\varepsilon_k + \frac{1}{2}U\right)\left(2L_z^{(k)} + 1\right) - U\left(\gamma K_+ + \gamma^* K_- + |\gamma|^2\right) . \qquad (2.13)$$

One can check from eq. (2.13) that the symmetry algebra of H_{ℓ}'' is $su(2) \oplus u(1)$ at half filling ($u(1) \oplus u(1)$ for $n \neq 1$), whereas the dynamical algebra is $g_d = g_d^{(0)} \oplus su(2)$. In view of the remaining steps of our scheme, it is indeed convenient to think of the latter $su(2)$ as generated by $\{e^{-i\varphi_{\gamma}}K_+ + e^{i\varphi_{\gamma}}K_-, e^{-i\varphi_{\gamma}}K_+ - e^{i\varphi_{\gamma}}K_-, K_z\}$. The set g is then given by $g = \{K_z, e^{-i\varphi_{\gamma}}K_+ - e^{i\varphi_{\gamma}}K_-\}$, whence $g' = g_d^{(0)} \cup \{e^{-i\varphi_{\gamma}}K_+ + e^{i\varphi_{\gamma}}K_-\}$, and $g_p \sim u(1)$ has a unique generator $e^{-i\varphi_{\gamma}}K_+ + e^{-i\varphi_{\gamma}}K_-$.

The only order parameter of the Hartree-Fock approach is therefore $|\gamma|$, in that $< e^{-i\varphi_{\gamma}}K_+ + e^{i\varphi_{\gamma}}K_- > = 2|\gamma|$. $|\gamma| \neq 0$ describes a phase for which the symmetries induced by K_z and $e^{-i\varphi_{\gamma}}K_+ - e^{i\varphi_{\gamma}}K_-$ are broken, namely a phase endowed with magnetic order. $|\gamma| = 0$ on the other hand provides a good description of the disordered phase, since equation (2.13) implies that the corresponding hamiltonian commutes with the whole $g_s^{(n)}$.

The BCS Approximation

The BCS bosonic linearization consists in introducing the "pairing" parameter $\delta \doteq < a_{i\downarrow}a_{i\uparrow} > \equiv |\delta|e^{i\varphi_{\delta}}$, whereby one replaces

$$n_{i\uparrow}n_{i\downarrow} \mapsto \delta \, a_{i\uparrow}^{\dagger}a_{i\downarrow}^{\dagger} + \delta^* a_{i\downarrow}a_{i\uparrow} - |\delta|^2 . \qquad (2.14)$$

The resulting linearized hamiltonian is

$$H_{\ell}''' = \sum_k \left[\varepsilon_k\left(2J_z^{(k)} + 1\right) + U\left(\delta J_+^{(k)} + \delta^* J_-^{(k)} - |\delta|^2\right)\right] , \qquad (2.15)$$

with

$$J_+^{(k)} \doteq a_{k\uparrow}^{\dagger}a_{-k\downarrow}^{\dagger} , \quad J_-^{(k)} \doteq a_{-k\downarrow}a_{k\uparrow} , \quad J_z^{(k)} \doteq \frac{1}{2}\left(n_{k\uparrow} + n_{-k\downarrow} - 1\right) . \qquad (2.16)$$

The dynamical algebra is $g_d = \oplus_k su(2)_k$, where each $su(2)_k$ is generated by $\{J_+^{(k)}, J_-^{(k)}, J_z^{(k)}\}$. We once more refer the latter $su(2)_k$ to a "rotated" basis $\{G_1^{(k)} \doteq i[\gamma_k J_z^{(k)} + \sigma_k S_+^{(k)}], G_2^{(k)} \doteq [\sigma_k J_z^{(k)} + \gamma_k S_+^{(k)}], G_3^{(k)} \doteq iS_-^{(k)}\}$, where $S_{\pm}^{(k)} \equiv$

$\frac{1}{2}\left(e^{i\varphi_\delta}J_+^{(k)} \pm e^{-i\varphi_\delta}J_-^{(k)}\right)$, with $\gamma_k = \cosh z_k$, $\sigma_k = \sinh z_k$, and $z_k = \tanh^{-1}(\zeta_k)$; being $\zeta_k \doteq \left(\frac{\varepsilon_k}{U|\delta|}\right)$. In such basis the hamiltonian (9) simply reads $H_\ell''' = 2U|\delta|$ $\sum_k\left\{\frac{1}{\gamma_k}G_2^{(k)} + \frac{1}{2}(\zeta_k - |\delta|)\right\}$. The set g is thus the collection of mutually commuting elements $g = \bigcup_k\{G_1^{(k)}, G_3^{(k)}\}$, and hence $g' = \bigcup_k\{G_2^{(k)}\}$. Since $g_d^{(0)}$ can be equally well be thought of as generated by $\bigcup_k\{J_z^{(k)}\}$, in this particular case it is manifestly a subalgebra of $g_d^{(I)}$, so that g_d coincides with $g_d^{(I)}$. Thus, finally, $g_p = \bigcup_k\{S_+^{(k)}\}$. The appropriate order parameter is hence just

$$\frac{1}{N_\Lambda}\sum_k <S_+^{(k)}> = \frac{1}{2N_\Lambda}\sum_i <e^{-i\varphi_\delta}a_{i\downarrow}a_{i\uparrow} + e^{i\varphi_\delta}a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger> \equiv |\delta| \quad . \qquad (2.17)$$

It is worth noticing that the order parameter here is unique because of the assumption, implicit in the self-consistency equation, that $\delta = <a_{i\downarrow}a_{i\uparrow}>$ is site-independent.

The phase described by $|\delta| \neq 0$ has the "superconductive" symmetry completely broken, whereas the whole "magnetic" symmetry survives.

On the other hand, when the order parameter $|\delta|$ equals zero, the linearized hamiltonian reduces to $H^{(0)}$, which is invariant with respect to the entire $g_s^{(n)}$ only for $n \neq 1$. Indeed, at $n = 1$, $H^{(0)}$ is invariant with respect to the subalgebra of $g_s^{(1)}$ $u(1) \oplus su(2)$, the whole symmetry $su(2) \oplus su(2)$ being recovered only for the unphysical case $\mu = 0$. Thus at half filling the vanishing of the order parameter $|\delta|$ restores only partially the "superconductive" symmetry, therefore it describes an *order-order* (and not an *order-disorder* transition), corresponding to the onset of non-vanishing pairing between couples of electrons. One should also point out that the self-consistent implementation of the present linearization scheme implies $U < 0$; in fact the self-consistency equation

$$|\delta| = \frac{1}{N_\Lambda}\sum_k \frac{\text{Tr}\{S_+^{(k)}\exp(-\beta H_\ell''')\}}{\text{Tr}\{\exp(-\beta H_\ell''')\}} \quad , \qquad (2.18)$$

has non-vanishing solutions for $|\delta|$ only if U is < 0. This latter feature is at the basis of the major interest devoted to the *negative-U* Hubbard model in the frame of high T_c superconductivity [67].

2.4.2 Fermionic Linearization Scheme

In this approach, the hopping term in (2.5) is linearized instead of the U term. Thus the approximate mean-field hamiltonian $H_\ell^{(F)}$ is particularly suited to describe the

system in the strong coupling limit, in which the electrons exhibit an almost atomic behavior (*i.e.* they are strongly localized).

$H_\ell^{(F)}$ has two interesting features: it has a dynamical algebra which is a super-algebra, and it can be diagonalized by a straighforward extension to the case of spectrum generating *superalgebras* of the (super)group-space Bogolubov rotation, turning out to be diagonal not in the wave vector Fock space but in the direct configuration space.

The linearization proceeds by replacing

$$\sum_{<i,j>} a_{i,\sigma}^\dagger a_{j,\sigma} \mapsto q \sum_i \left(\bar{\vartheta}_\sigma i\sigma + a_{i,\sigma}^\dagger \vartheta_\sigma - \bar{\vartheta}_\sigma \vartheta_\sigma \right) \quad , \qquad (2.19)$$

where q denotes the number of nearest neighbours per site in Λ, whereas $\vartheta_\sigma = < i\sigma >$ is assumed site independent. $\bar{\vartheta}_\sigma, \vartheta_\sigma$ belong to the odd sector of a Grassmann-like algebra.

The detailed analysis of the Hubbard model within this scheme will be presented in the next sections of this chapter. Here, let us just mention that the dynamical algebra is the direct sum of N_Λ copies of the same superalgebra: $g_d = \bigoplus_i u(2|2)_i$ and the order parameters turns out to be proportional to $(\vartheta_\uparrow \bar{\vartheta}_\uparrow + \vartheta_\downarrow \bar{\vartheta}_\downarrow)$, and to $\vartheta_\downarrow \bar{\vartheta}_\uparrow + \vartheta_\uparrow \bar{\vartheta}_\downarrow$. Notice that once more, due to the assumed translational invariance of the ϑ_σ's the two order parameters are site-independent.

In the case when also spin-exchange invariance is assumed (*i.e.* $\vartheta_\uparrow \equiv \vartheta_\downarrow$), g_d reduces [55] to $\bigoplus_i (u(1|1) \oplus u(1|1))_i$ and the two parameters coalesce into a single one, say $\vartheta\bar{\vartheta}$. In this case the corresponding self-consistency equation has solutions $\vartheta\bar{\vartheta} = 0$, describing a disordered phase in which the whole $g_s^{(n)}$ symmetry is restored, as well as $\vartheta\bar{\vartheta} \neq 0$. In the latter case the original symmetry is completely broken (both the "superconducting" and the "magnetic" $su(2)$). As the order parameter is unique, in general it will describe a superposition of the two ordered phases ("mixed" phase). Of course, in the more general case when $\vartheta_\uparrow \neq \vartheta_\downarrow$ one expectes that the existence of two order parameters might lead to a deeper insight in the structure of the ordered phases.

The global $SO_4 = (SU_2 \otimes SU_2)/\mathbb{Z}_2$ symmetry discussed by Yang and Zhang may be thought of – as pointed out by the same authors – as related to the possible coexistence of "superconductive" and "magnetic" phase. We have seen how the standard bosonic linearization allows one to define order parameters describing the breaking of one symmetry only at a time. On the contrary, the fermionic linearization scheme leads to introducing order parameters which break both symmetries simultaneously, and are therefore able to represent "mixed" phases. In particular, such a scheme

is the only one permitting to describe a phase with $U > 0$, characterized by an order parameter associated with the breaking of the superconductive symmetry. It is worth pointing out here that even though states non conserving the local average number of electrons may thus be generated, such states do not correspond to non-vanishing pairing, which can indeed be obtained only from extended Hubbard models [55, 20]

An important characteristic feature which emerged from this analysis is the property that even within a linearized scheme the transition from an ordered to a disordered phase can be consistently described only if the whole original symmetry is restored for the linearized hamiltonian by the vanishing of the order parameters. This is not always the case in the bosonic mean field approximations: when it happens, it leads to situations which are of very little physical relevance (the self-energy term becomes identically zero). Therefore, the fermionic mean field approach on the other hand allows us to restore the complete symmetry in the disordered phase in a non-trivial dynamical way.

2.5 The n-cluster Fermi-linearized Hubbard model

In this section, by means of an interacting cluster expansion method to be defined below, we apply the Fermi-linearization scheme dicussed in Chapter 2 to a variant of the Hubbard model

$$H_H = \sum_{i \in \Lambda} \sum_{\sigma} \varepsilon_i n_{i\sigma} + \sum_{i \in \Lambda} U_i n_{i\uparrow} n_{i\downarrow} + \sum_{<i,j>} t_{ij} \sum_{\sigma,\sigma'} a_{i\sigma}^\dagger a_{j\sigma'} \qquad (2.20)$$

where Λ is a d-dimensional lattice of N sites and $i \in \Lambda$ is the site label. As usual, the sum over $< i, j >$ is meant to run over all the sites i and j of Λ which are nearest neighbors.

Let $\{H_n / n \leq N\}$ be a sequence of hamiltonians which approximate $H = \sum_{\{c_n\} \in \Lambda} H_n$, where $\{c_n\}$ denotes any possible cluster covering of Λ. The cluster linearization method consists in taking into account exactly the mutual interactions of the particles within the selected cluster and using fermionic linearization to describe interactions between neighbouring clusters [56].

In the model described by (2.20), one can recover the standard Hubbard model by choosing the spin-flip amplitude $t_{\sigma,-\sigma} = 0$. On the contrary, we select $t_{\sigma,-\sigma} = t_{\sigma,\sigma} = t$ and this naturally leads to introducing the new set of local operators

$$A_i = \frac{1}{\sqrt{2}} (a_{i\uparrow} + a_{i\downarrow}) \quad , \quad N_i = A_i^\dagger A_i$$

$$D_i = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} + a_{i\uparrow}a_{i\downarrow}^\dagger + a_{i\downarrow}a_{i\uparrow}^\dagger) \quad , \quad D_i^2 = D_i. \tag{2.21}$$

Notice that the operators $A_i, A_i^\dagger$ and N_i satisfy the same commutation and anti-commutation relations as $a_i, a_i^\dagger$ and n_i and that D_i commute with both $A_j, A_j^\dagger$ and N_j.

In terms of the old operators, we have the relations

1. $N_i + D_i = \sum_\sigma n_{i\sigma}$;

2. $N_i D_i = n_{i\uparrow} n_{i\downarrow}$;

3. $N_i = \frac{1}{2}\sum_\sigma (n_{i\sigma} + a_{i\sigma}^\dagger a_{i,-\sigma})$.

Through the new operators (2.21), the hamiltonian (2.20) can be rewritten as

$$H \equiv H_{\{\Lambda\}} = \sum_{i\in\Lambda}(\varepsilon_i + UD_i)N_i + t\sum_{<i,j>}(A_iA_j^\dagger + A_jA_i^\dagger) + \sum_{i\in\Lambda}\varepsilon_i D_i \tag{2.22}$$

and explicit reference to the spin index has now disappeared.

In this case, the fermionic linearization acts on the hopping interactions between sites on the cluster boundary and sites outside the cluster replacing the bilinears by the linear form

$$A_i^\dagger A_j \to \bar\eta_i A_j + A_i^\dagger \eta_j - \bar\eta_i\eta_j. \tag{2.23}$$

As discussed in section (1.2.2), the coefficients $\bar\eta_i = < A_i^\dagger >$ and $\eta_j = < A_j >$ belong to the odd sector $\mathcal{G}_1$ of the non-associative $\mathbb{Z}_2$ Grassmann-like graded algebra $\mathcal{G} = \mathcal{G}_0 \oplus \mathcal{G}_1$. Non associativity raises from the physical requirement that $\eta_i^2 = 0$ but $(\eta_i\eta_j)^2 \neq 0$. H_n is then given by ($\tau := t(n-1)$):

$$H_n = \sum_{\alpha=1}^{n} H_\alpha^{(l)} + \tau \sum_{\substack{\alpha=1 \\ (\text{mod } n)}}^{n} (A_\alpha^\dagger A_{\alpha+1} + A_{\alpha+1}^\dagger A_\alpha) \tag{2.24}$$

with

$$H_\alpha^{(l)} = \epsilon_\alpha(N_\alpha + D_\alpha) + U_\alpha D_\alpha N_\alpha + \sqrt{2}(\vartheta_\alpha A_\alpha + A_\alpha^\dagger \bar\vartheta_\alpha) - C_\alpha \tag{2.25}$$

and

$$\vartheta_\alpha := t\sum_{k\in\Lambda/c_n} \bar\eta_k - t\sum_{\gamma=1}^{n} \bar\eta_\gamma \tag{2.26}$$

$$C_\alpha := \frac{\tau}{2}\sum_{k\in\Lambda/c_n} (\bar\eta_\alpha\eta_k + \bar\eta_k\eta_\alpha) - \tau\sum_{\gamma=1}^{n} \bar\eta_\alpha\eta_\gamma \tag{2.27}$$

where $k = \text{n.n.}(\alpha)$.

As we are interested here only in the spectrum of the hamiltonian and in the zero temperature features of the model, it is irrilevant which covering one selects (whereas at $T \neq 0$ one should consider all possible coverings of the lattice in order to account properly for the global lattice entropy). It is worth to point out that the trimer is the minimal cluster necessary to obtain a complete covering of the decorated lattice typical of Copper-Oxide planes in high-T_c superconductors.

It is now straighforward to show that the dynamical algebra associated with the n-cluster model hamiltonian H is $\mathcal{S}_n = \oplus_1^{2^n} u(n|1)$ where the superalgebra $u(n|1)$ is generated by $(n+1)^2$ elements, (n^2+1) of which form the bosonic sector $\mathcal{B}(u(n|1))$ and $2n$ are in the fermionic sector $\mathcal{F}(u(n|1))$. More explicitly:

$$\mathcal{B}(u(n|1)) = \{\mathbb{I}, A_i^\dagger A_j;\ i,j \in c_n\} \sim u(n) \oplus u(1) \qquad (2.28)$$

$$\mathcal{F}(u(n|1)) = \{A_i, A_i^\dagger;\ i \in c_n\}. \qquad (2.29)$$

As the D_i's are projectors, the 2^n orthogonal copies of $u(n|1)$ which generate $\mathcal{S}_n$ are labelled by the 2^n possible different combinations of eigenvalues $d_i \in \{0,1\}$ of D_i ($i \in c_n$). From now on, we indicate with a multiindex λ one of these combinations and we denote by $\mathcal{L}$ the set of all the possible λ's, whereas P_λ is the projection operator on the subspace $u(n|1)_\lambda$ associated with the given λ. Therefore $H_c = \sum_{\lambda \in \mathcal{L}} H_\lambda \equiv \sum_{\lambda \in \mathcal{L}} H_c P_\lambda$. In order to obtain the spectrum of H_c, we apply a generalized Bogolubov rotation in the (super)group space, which in turn can be implemented by the adjoint action of a suitable operator $Z \in \mathcal{S}_n$.

With no loss of generality, we write

$$\exp Z = \exp Z^{(b)} \exp Z^{(f)} \qquad (2.30)$$

where, due to the direct product sum structure of $\mathcal{S}_n$, we can set

$$Z^{(b)} = \sum_{\lambda \in \mathcal{L}} Z_\lambda^{(b)} \equiv \sum_{\lambda \in \mathcal{L}} \sum_{\substack{\alpha=1 \\ (\text{mod } n)}}^n z_\alpha^{(\lambda)}(A_\alpha^\dagger A_{\alpha+1} - A_{\alpha+1}^\dagger A_\alpha) \qquad (2.31)$$

$$Z^{(f)} = \sum_{\lambda \in \mathcal{L}} Z_\lambda^{(f)} \equiv \sum_{\lambda \in \mathcal{L}} \sum_{\alpha=1}^n (\xi_\alpha^{(\lambda)} A_\alpha + \bar{\xi}_\alpha^{(\lambda)} A_\alpha^\dagger) \qquad (2.32)$$

with $\{z_\alpha^{(\lambda)}/\lambda \in \mathcal{L},\ \alpha = 1,\ldots,n\} \in \mathcal{G}_0$, $\{\xi_\alpha^{(\lambda)}/\lambda \in \mathcal{L},\ \alpha = 1,\ldots,n\} \in \mathcal{G}_1$. The diagonal form $\mathcal{H}$ of H_c can then be obtained from

$$\mathcal{H} = \bigoplus_{\lambda \in \mathcal{L}} \exp(\text{ad } Z_\lambda^{(b)})(\exp(\text{ad } Z_\lambda^{(f)})(H_\lambda)$$

$$= \bigoplus_{\lambda \in \mathcal{L}} \exp \left(\mathrm{ad} \ Z_\lambda^{(b)} \right) (\mathcal{H}_\lambda^{(f)}) \tag{2.33}$$

by suitably choosing the coefficients $z_\alpha^{(\lambda)}$ and $\xi_\alpha^{(\lambda)}$ in such a way that the resulting operator belongs to the Cartan subalgebra of $\mathcal{B}(\mathcal{S}_c)$. The first step consists in selecting the variables $\{\xi_\alpha^{(\lambda)}\}$ in such a way that $\mathcal{H}_\lambda^{(f)}$ lives in $\mathcal{B}(\mathcal{S}_c)$ and this leads in general to a system of linear equations (homogeneous over the odd sector $\mathcal{G}_1$ of $\mathcal{G}$ and hence equivalent to a regular linear system over $\mathbb{R}$).

Notice that due to the presence of the anticommuting Grassmann-like coefficients for the fermionic operators, we have

$$[\ \eta_\alpha F_\alpha \ , \ \eta_\beta F_\beta \ ] \ = \ \eta_\beta \eta_\alpha \{\ F_\alpha \ , \ F_\beta \ \} \ , \quad \eta_\alpha, \eta_\beta \in \mathcal{G}_1 \ , \tag{2.34}$$

$$[\ \eta F \ , \ \alpha B \ ] \ = \ \alpha \eta [\ F \ , B \ ] \ , \quad \alpha \in \mathcal{G}_0, \eta \in \mathcal{G}_1 \tag{2.35}$$

and therefore we remain into the superalgebra.

After this, since we know that the bosonic sector of a superalgebra is a Lie algebra, we can perform a usual Bogolubov rotation in $\mathcal{B}(\mathcal{S}_c) \equiv u(n) \oplus u(1)$ with the adjoint action of $Z^{(b)}$ as seen in section (1.3).

2.6   The single-site cluster

2.6.1   The spectrum

The simplest case, which we will work out in detail in this section, is obviously the *single-site* cluster, which is equivalent to a mean-field treatment. Let us rewrite the Hubbard hamiltonian for this particular case in the following form:

$$H_H = \sum_{i,\sigma} \varepsilon_i n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + \sum_{<i,j>\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}. \tag{2.36}$$

Upon defining

$$\vartheta := \vartheta_{i\sigma} = \sum_{j=n.n.(i)} t_{ji} < a_{j\sigma}^\dagger > \in \mathcal{G}_1; \tag{2.37}$$

and assuming further that $\vartheta_{i\uparrow} = \vartheta_{i\downarrow}$ (time reversal invariance), and that $\varepsilon_i = \varepsilon_{i\sigma}$ is independent of σ, the linearized hamiltonian takes the form $H_H^{(lin)} = \sum_i H^{(i)}$ with

$$H^{(i)} = \varepsilon(n_+ + n_-) + U n_+ n_- + \vartheta(a_+ + a_-) - \bar\vartheta(a_+^\dagger + a_-^\dagger) \tag{2.38}$$

where we dropped the index i and wrote $\pm$ for $\uparrow, \downarrow$.

$H^{(i)}$ is an element of a superalgebra $\mathcal{S}_i$, hence $H_H^{(lin)} \in \mathcal{S} = \oplus_i \mathcal{S}_i$. $\mathcal{S}_i$ is the 16-dimensional superalgebra $u(2|2)$ which can be thought of as the extension , by the Cartan element n_+n_-, of $su(2|2)$. To be more precise, $H^{(i)}$ sits in a smaller superalgebra $\mathcal{A} = \mathcal{B}_\mathcal{A} \oplus \mathcal{F}_\mathcal{A}$ generated by

$$\mathcal{B}_\mathcal{A} = \{n_+ + n_-, \; n_+n_-, \; a_+^\dagger a_- + a_-^\dagger a_+, \; \mathbb{I}\} \; , \tag{2.39}$$

$$\mathcal{F}_\mathcal{A} = \{a_+ + a_-, \; a_+^\dagger + a_-^\dagger, \; n_+a_- + n_-a_+, \; n_+a_-^\dagger + n_-a_+^\dagger\} \; , \tag{2.40}$$

which is an 8-dimensional subalgebra of $\mathcal{S}_i$. $\mathcal{A}$ is isomorphic to the centralizer $C_D u(2|2) = u(1|1) \oplus u(1|1)$, where $D = (n_+ + n_- + a_+a_-^\dagger + a_-a_+^\dagger)$. However, $\mathcal{A}$, unlike $\mathcal{S}_i$, does not contain in its bosonic sector the Lie subalgebra $su(2)$ necessary to rotate $H^{(i)}$ to diagonal form in Fock space.

Now, we perform the diagonalization with the two-step procedure introduced in the last section. First consider the adjoint action of the skew hermitian fermionic element $Z^{(f)} \in \mathcal{F}(\mathcal{S}_i)$,

$$Z^{(f)} := \lambda(a_+ + a_-) + \mu(n_+a_- + n_-a_+) - \text{ h.c.}, \tag{2.41}$$

on $H^{(i)}$, where $\lambda, \mu \in \mathcal{G}_1$. Selecting $\lambda = -\vartheta/\varepsilon$ and $\mu = c\vartheta$, $c = U/\varepsilon(U + \varepsilon)$, this rotates $H^{(i)}$ into H_b which no longer contains fermionic terms. The second step consists to rotate H_b into H_0 which is diagonal in the Fock basis $\{|n_+ > \oplus |n_- > ; n_\pm \in \mathbb{Z}_2\}$ by the adjoint action of the bosonic operator

$$Z^{(b)} := \varphi(a_+a_-^\dagger - a_-a_+^\dagger) \tag{2.42}$$

which lies in $\mathcal{S}_i/\mathcal{A}$. By selecting $\varphi = (2m + 1)\frac{\pi}{4}$, $m \in Z$, we obtain:

$$\exp(\text{ad } Z^{(b)})\exp(\text{ad } Z^{(f)}) \, H^{(i)} := H_0 \tag{2.43}$$

with

$$H_0 = \varepsilon(n_+ + n_-) + Un_+n_- + 2c\vartheta\bar{\vartheta}n_{(-1)^{m+1}} - \frac{2}{\varepsilon}\vartheta\bar{\vartheta}. \tag{2.44}$$

Notice that $\vartheta\bar{\vartheta} \in \mathcal{G}_0$ and the spectrum is obviously independent of the choice of the integer m.

2.6.2 The self-consistency equations

We now compute statistical-mechanical averages in the canonical ensemble. With $Z := \text{tr}\{\exp[-\beta H^{(i)}]\}$, we obtain

$$< \hat{O} > := Z^{-1} \, \text{tr}\{\hat{O} \exp [-\beta H^{(i)}]\} \tag{2.45}$$

$$= \frac{\text{tr}\{\exp(-\beta H_0)\exp(\text{ad } Z^{(b)})(\exp(\text{ad } Z^{(f)})(\hat{O}))\}}{\text{tr}\{\exp(-\beta H_0)\}}$$
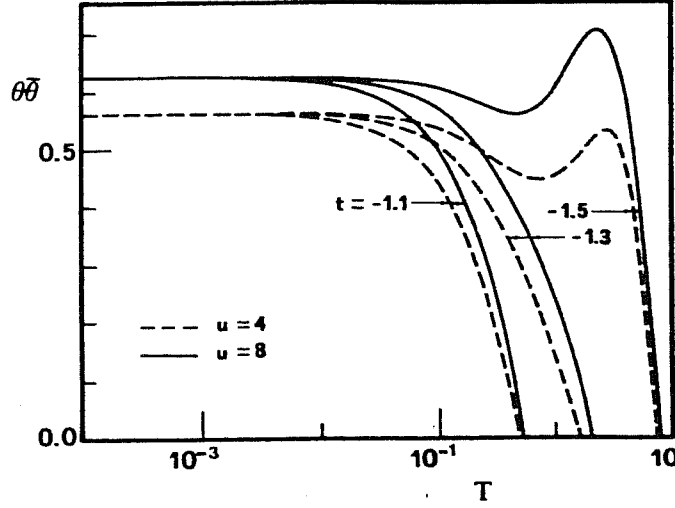
Figure 2.1: $\vartheta\bar{\vartheta}$ vs. T (semilogarithmic scale). Notice that T_c depends strongly on t and weakly on U.

where $\beta = (k_B T)^{-1}$, k_B denoting the Boltzmann's constant. The model defined by (2.38) has no *superconductive* order parameter, in that $< a_+ a_- >$ is identically zero. However it does have a *magnetic* order parameter which is interesting to consider. We evaluate first

$$\exp(\text{ad } Z^{(b)})(\exp(\text{ad } Z^{(f)})\ [\vartheta(a_+ + a_-)]) \tag{2.46}$$

$$= 2\vartheta\bar{\vartheta}\{-\frac{1}{\varepsilon} + cn_{(-1)^{m+1}}\} + \sqrt{2}\vartheta(-1)^{[\frac{m+1}{2}]}a_{(-1)^m} \tag{2.47}$$

whence, recalling that a_+, a_- have vanishing trace in the basis in which H_U is diagonal,

$$< \vartheta(a_+ + a_-) >= -\frac{2\vartheta\bar{\vartheta}}{\varepsilon(U + \varepsilon)}\{\varepsilon + \frac{U}{\mathcal{Z}_r}[1 + \exp(-\beta\varepsilon)\} \tag{2.48}$$

where

$$\mathcal{Z}_r = 1 + \exp(-\beta\varepsilon) + \exp(-2\beta c\vartheta\bar{\vartheta})[\exp(\beta\varepsilon) + \exp(-\beta(2\varepsilon + U))] \tag{2.49}$$

is the *reduced* partition function. Self-consistency is imposed by requiring that (2.37) is satisfied. For example in the case in which complete n.n. symmetry is assumed, it reads $< a_+ + a_- >= 2\bar{\vartheta}/t$. Notice that in this case the result no longer depends

on the dimensionality. Upon setting

$$\kappa := \frac{(U + \varepsilon)(t + \varepsilon)}{tU}, \tag{2.50}$$

one gets

$$\vartheta\bar{\vartheta} = -\frac{1}{2\beta c}\ln\left\{\frac{\kappa[1 + \exp(-\beta\varepsilon)]}{(1 - \kappa)\exp(-\beta\varepsilon)[1 + \exp(-\beta(U + \varepsilon))]}\right\}, \tag{2.51}$$

for $\beta > \beta_c$ and $\vartheta\bar{\vartheta} = 0$ for $\beta < \beta_c$, where β_c is the solution of the equation

$$\frac{1 + \exp(-\beta_c(U + \varepsilon))}{1 + \exp(\beta_c\varepsilon)} = \frac{\kappa}{1 - \kappa}. \tag{2.52}$$

Figure(2.1) shows a plot of $\vartheta\bar{\vartheta}$ vs. T ($T_c := (k_B\beta_c)^{-1}$). One can see that $\vartheta\bar{\vartheta}$ has indeed the features of a magnetic order parameter.

2.7 The dimer-cluster approximation

2.7.1 The dynamical algebra

We now consider the next high order approximation after the mean-field one, namely the two-site cluster (dimer). The dimer cluster can be constructed whenever the lattice Λ can be assumed to be the disjoint union of the two sublattices, $\Lambda = \Lambda_1 \cup \Lambda_2$ such that the sites of each have all their nearest neighbours in the other. From equations (2.24) and (2.25) we can write down immediately the linearized hamiltonian as

$$H_c = H_1^{(l)} + H_2^{(l)} + t(A_1^\dagger A_2 + A_2^\dagger A_1) \tag{2.53}$$

with

$$\begin{aligned}
H_\alpha^{(l)} &= \varepsilon_\alpha(N_\alpha + D_\alpha) + U_\alpha D_\alpha N_\alpha + \sqrt{2}(\vartheta_\alpha A_\alpha + A_\alpha^\dagger \bar{\vartheta}_\alpha) \\
&+ \sum_{i \text{ n.n.}(\alpha)\neq\bar{\alpha}} \frac{t}{2}(\bar{\eta}_\alpha\eta_i + \bar{\eta}_i\eta_\alpha) - t\bar{\eta}_\alpha\eta_{\bar{\alpha}}
\end{aligned} \tag{2.54}$$

and

$$\vartheta_\alpha := \sum_{\substack{i \text{ n.n.}(\alpha) \\ i\neq\bar{\alpha}}} t(\bar{\eta}_i - \bar{\eta}_{\bar{\alpha}}) \quad . \tag{2.55}$$

For the sake of simplicity, but with no substantial loss of generality, it has been assumed in (2.53) that the hopping coupling between the two sublattices Λ_1 and Λ_2 is spin-independent because the possible diversity in the two amplitudes can be embodied into the normalization of the ϑ_α in (2.55).

From the general discussion, we deduce that H_c is an element of the superalgebra $\mathcal{S}_c = u(2|1) \oplus u(2|1) \oplus u(2|1) \oplus u(2|1)$. Each $u(2|1)$ is itself a superalgebra generated by nine elements, five in $\mathcal{B}(u(2|1))$ and four in $\mathcal{F}(u(2|1))$:

$$\begin{aligned}
\mathcal{B}(u(2|1)) &= \{\mathbb{I}, A_1^\dagger A_1, A_2^\dagger A_2, A_1^\dagger A_2, A_2^\dagger A_1\}, \\
\mathcal{F}(u(2|1)) &= \{A_1, A_1^\dagger, A_2, A_2^\dagger\}.
\end{aligned} \tag{2.56}$$

The four orthogonal copies of $u(2|1)$ which generate the whole $\mathcal{S}_c$ can be obtained by multiplying the odd and the even sectors of $u(2|1)$ successively by the four idempotent elements in the center $\mathcal{C}$ of $\mathcal{S}_c$:

$$\begin{aligned}
\mathcal{P}_1 &\equiv (1 - D_1)(1 - D_2) & , \quad \mathcal{P}_2 &\equiv D_1(1 - D_2) \\
\mathcal{P}_3 &\equiv (1 - D_1)D_2 & , \quad \mathcal{P}_4 &\equiv D_1 D_2
\end{aligned} \tag{2.57}$$

where the operators D_i were defined in (2.21).

It is worth noticing that $\mathcal{S}_c$ is a subalgebra of $su(4|4)$, which contains the graded algebra necessary to perform the generalized Bogolubov transformation for the diagonalization of H_c in Fock space.

What makes this particular model interesting is that even though there are still only two primitive order paramaters ϑ_1, ϑ_2 avalaible to describe the theory, and two self-consistency equations which determine them as a function of the temperatiure , the model exhibits a *pairing phase* in addition to the previous magnetic one. More precisely, in a phase for which $\vartheta_\alpha \bar\vartheta_\alpha$ is not identically zero for both $\alpha = 1, 2$, we would find that

1. $< a_{1\sigma} a_{2\sigma'}^\dagger > = < a_{2\sigma'} a_{1\sigma}^\dagger >^* \neq 0 \quad \forall \sigma, \sigma'$, since it is proportional to $\vartheta_1 \bar\vartheta_2$;

2. $| < a_{1\sigma} a_{2\sigma'} > | \neq 0$ and $| < a_{\alpha\sigma} a_{\alpha\sigma'}^\dagger > | \neq 0 \quad \forall \sigma, \sigma'$ and $\forall \alpha$, in that they are proportional to $(|\vartheta_1 \bar\vartheta_1 \vartheta_2 \bar\vartheta_2|)^{1/2}$ and $\vartheta_\alpha \bar\vartheta_\alpha$ respectively.

In other words, the model appears to show a simultaneous antiferromagnetic and superconductive phase transition.

2.7.2   The ground state

Let us define a generic supercoherent state $| \psi_J >$ [2] as

$$|\psi_J > = \mathcal{U} \mid \omega >_c, \quad \mathcal{U} := \exp(Z), \quad Z = -Z^\dagger \in \mathcal{S}_c \tag{2.58}$$

---

[2] See appendix C for details

where $\mid \omega >_c$ is the *heighest weight vector* of $\mathcal{S}_c$. If $\exp(\mathrm{ad}Z)(H_c)$ is diagonal, then $\mid \omega >_c$ coincides with the vacuum of H_c. In this case, we will identify the dimer-cluster ground state $\mid \psi_G >$ with that particular supercoherent state which minimizes the system internal energy (namely the expectation value of H_c), for the appropriate value of the chemical potential μ at fixed site occupancy.

Here we sketch the main steps of the computation while details can be found in [55]. Using formulas (2.30),(2.31) and (2.32) with $n = 2$, the $T = 0$ ground state of the model will correspond to the particular choice of the twelve parameters $\{\ z^{(\lambda)},\ \xi_\alpha^{(\lambda)} \mid \lambda = 1,\ldots,4 \ ; \ \alpha = 1,2\}$ and μ for which

1. all the derivatives of $\mathcal{H} \equiv < \psi_f \mid H_c - \mu N_c \mid \psi_f >$ with respect to the parameters $\{z^{(\lambda)}, \xi_\alpha^{(\lambda)}\}$ are equal zero, where N_c is the total number of particles operator for the dimer.

2. $< \psi_f \mid N_c \mid \psi_f >= n_0$, where n_0 is the fixed dimer occupation number.

3. η_α is identified with the average $< a_{\alpha\sigma} >$.

Noticing that $\mathcal{H}$ contains only bilinear products of elements of $\mathcal{G}_0$, since the only elements of $\mathcal{G}_1$ entering the model are ϑ_1 and ϑ_2, the parameters $\xi_\alpha^{(\lambda)}$ have to be linear combinations of the ϑ_β's. Upon the reparametrization $\xi_\alpha^{(\lambda)} = \kappa_\alpha^{(\lambda)}\vartheta_{\alpha+1}$, which allows transforming the derivatives with respect to $\xi_\alpha^{(\lambda)}$ into usual derivatives with respect to $\kappa_\alpha^{(\lambda)}$, $\mathcal{H}$ does contain (linearly) only elements of $\mathcal{G}_0$ of the form $\vartheta_\alpha\bar{\vartheta}_\alpha$ and $\vartheta_\alpha\bar{\vartheta}_{\alpha+1}$.

A possible realization of the elements of $\mathcal{G}_1$ comes from the identification of the product in $\mathcal{G}$ with the inner product over the vector (super-) space associated with $\mathcal{G}$ itself. The latter can be defined in terms of any antisymmetric function of the phase associated with its factors. Here we will assume

$$\eta_i\eta_j \equiv \sin(\varphi_i - \varphi_j) \quad , \tag{2.59}$$

where φ_i has to be determined consistently with the relation $\eta_i\bar{\eta}_i \equiv \sin(2\varphi_i)$.

From (2.59), we deduce that $\bar{\vartheta}_\alpha\vartheta_\alpha \sim \sin(2\varphi_{\alpha+1})$ and $\bar{\vartheta}_\alpha\vartheta_{\alpha+1} \sim \sin(\varphi_\alpha + \varphi_{\alpha+1})$. Including the self-consistency equations related to this fundamental bilinears in the minimization scheme as constraints with the introduction ot two new Lagrange multipliers ρ_1,ρ_2, there finally results a system of seventeen equations in the seventeen unknowns $\{z^{(\lambda)}, \kappa_\alpha^{(\lambda)}, \mu, \varphi_\alpha, \rho_\alpha \mid \lambda = 1,\ldots,4 \ ; \ \alpha = 1,2\}$. The solutions of this system allows us to evaluate, at the ground state, the rotation paramaters $\{\tilde{\kappa}_\alpha^{(\lambda)}\tilde{z}^{(\lambda)}\}$ and in particular the pairing order parameter

$$\mathcal{P} \equiv 2 \,\mathrm{Re}\, (< A_1 A_2 > - < A_1 >< A_2 >). \tag{2.60}$$
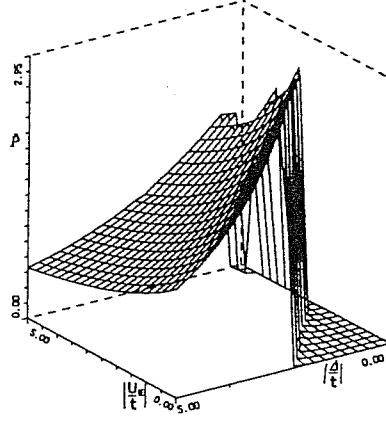
Figure 2.2: $\mathcal{P}$ vs. $|U_1/t|$ and $|\Delta/t|$ for $n_0 = 1.5$

Besides particular solutions corresponding to zero pairing, the system has another set of solutions which exhibit non-zero pairing and should be computed numerically. We report below the results obtained in [55] for the case $U_2 = 0$, $q_1 = q_2 = 4$.

Figures 2.2 and 2.3 show, for $n_0 = 1.5$ and $n_0 = 0.5$ respectively, the pairing $\mathcal{P}$ versus $|U_1/t|$ and $|\Delta/t|$ with both U_1 and Δ positive and t negative. One can check from the figures how the first quadrant of the phase-space (U_1, Δ), the domain where $\mathcal{P} = 0$ consists roughly of a triangle in the proximity of the origin whose area increases with decreasing n_0 (all the lines separating the phase with $\mathcal{P} = 0$ from that with non-zero pairing, upper sides of the triangles, converge to the same point for $\Delta = 0$ ($|U_1/t| \simeq 2$)). Everywhere else the pairing is differen from zero, and smoothly decreases asymptotically to zero for very large $|U_1/t|$. A finer numerical analysis also shows the existence of an intermediate phase with pairing very small but not zero. The transition from the phase $\mathcal{P} = 0$ to the latter is smooth, whereas the transition from the intermediate phase to that with large $\mathcal{P}$ is discontinuous. There is some numerical evidence to the effect that such a transition may occur as well for large $|\Delta/t|$, at least for low $|U_1/t|$ (see figure 2.3).

These results strongly support the conjecture that the cluster fermionic linearization method allows quantitatively describing a phase with spatial electron pairing, such as that typical of high-T_c superconductors, in terms of Hubbard-like models.
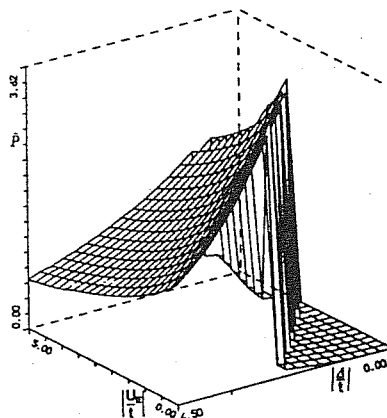
Figure 2.3: $\mathcal{P}$ vs. $|U_1/t|$ and $|\Delta/t|$ for $n_0 = 0.5$

2.8 Supersymmetric extensions of the Hubbard model

In this section we shall deal with $d = 2$ only, showing how in this case, there is a particular class of superlattices of the sort introduced in section(2.7) naturally lending themselves to the construction of new hamiltonians which are supersymmetric (whether or not the supersymmetry is exact or spontaneously broken depends on the ground state). The conserved fermionic supercharges whereby the hamiltonians are constructed are elements of the fermionic sector of the dynamical superalgebras introduced in section(2.7), or obvious generalizations thereof.

It is interesting to point out that the structure of a lattice realizing the above conditions is indeed that of most of the known compounds (essentially copper oxides with different rare earth additions, all appearing as a stack of weakly coupled two-dimensional planes of Cu and O atoms) exhibiting high-T_c superconductive phase transitions.

Let Λ_2 be a $2-d$ square lattice, whose sites are labelled by pairs of integers $(i \mid j)$ denoting their cartesian coordinates in units of lattice spacings, with the property that

(a) (odd—odd) :   empty site   ;

(b) (odd—even) : $\bullet$ site   ;

(c) (even—even): $\circ$ site   .
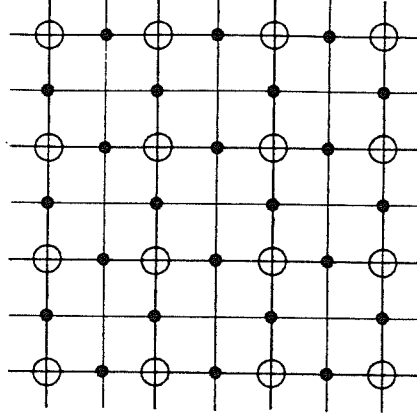
Figure 2.4: The lattice Λ_2

Such a lattice is shown schematically in figure 2.4.

We now construct the generic fermionic charge $Q \in \mathcal{F}(\cup_c \mathcal{F}(u(4|4)_c))$

$$
\begin{aligned}
Q = \sum_{\substack{i,j=0 \\ (\text{mod } 2)}} \sum_{\sigma} \Big\{ & [n_{(i,j),\sigma} \sum_{\sigma'} [\alpha_{\sigma'}(a_{(i,j\pm1),\sigma'} + a_{(i\pm1,j),\sigma'}) + \text{h.c.}] \\
& + [\, \beta_\sigma(n_{(i,j+1),\sigma} a_{(i,j+1),-\sigma} + n_{(i+1,j),\sigma} a_{(i+1,j),-\sigma}) + \text{h.c.}] \\
& + [\, \lambda_\sigma a_{(i,j),\sigma} + \mu_\sigma(a_{(i+1,j),\sigma} + a_{(i,j+1),\sigma}) + \text{h.c.} \,] \Big\} \quad ; \qquad (2.61)
\end{aligned}
$$

where $\alpha_\sigma, \beta_\sigma, \lambda_\sigma, \mu_\sigma$ and their conjugates are complex numbers yet to be determined in such a way as to get the desired hamiltonian.

In the following, we will assume Q hermitian ($Q^\dagger = Q$ and $H = Q^2$) and analize two particular cases corresponding to the following choices of the parameters:

1. $\beta_\sigma = i\kappa\alpha_{-\sigma}$ with $\kappa \in \mathbb{R}$;

2. the phase of β_σ equals the phase of α_σ and α_σ is site(o)-dependent with $\alpha_\sigma(l|j) = \exp(i\frac{\pi}{4}(l+j))\alpha_\sigma$, where $\alpha_\sigma \equiv \alpha_\sigma(0|0)$ (and analogously for β_σ).

In case (1), the resulting hamiltonian is

$$
H_{(1)} = \sum_{\substack{i,j=0 \\ (\text{mod } 2)}} \sum_{\sigma} \sum_{l=1}^{7} \mathcal{H}_{(i|j),\sigma}^{(l)} \qquad (2.62)
$$

where

$$\mathcal{H}^{(1)}_{(i|j),\sigma} = \underbrace{\sum_{\sigma'}(2|\alpha_{\sigma'}|^2 + \alpha_{\sigma'}\mu^*_{\sigma'} + \alpha^*_{\sigma'}\mu_{\sigma'})}_{\equiv \epsilon_\circ} n_{(i,j),\sigma} \tag{2.63}$$

is the self-energy of o-sites;

$$\mathcal{H}^{(2)}_{(i|j),\sigma} = \underbrace{(\beta_\sigma\bar{\mu}_{-\sigma} + \bar{\beta}_\sigma\mu_{-\sigma} + |\beta_\sigma|^2)}_{\equiv \epsilon_\bullet}(n_{(i,j\pm1),\sigma} + n_{i\pm1,j),\sigma}) \tag{2.64}$$

is the self-energy of •-sites;

$$\mathcal{H}^{(3)}_{(i|j),\sigma} = \underbrace{\left(\sum_{\sigma'}4|\alpha_{\sigma'}|^2\right)}_{\equiv U} n_{(i,j),\uparrow}n_{(i,j),\downarrow} \tag{2.65}$$

is the on-site Coulomb repulsion at o-sites;

$$\mathcal{H}^{(4)}_{(i|j),\sigma} = \sum_{\sigma'}\underbrace{(\alpha^*_\sigma\alpha_{\sigma'} + \alpha_\sigma\alpha^*_{\sigma'})}_{\equiv V^{(\sigma,\sigma')}} n_{(i,j),\sigma}(n_{(i,j\pm2),\sigma'} + n_{(i\pm2,j),\sigma'}) \tag{2.66}$$

is the Coulomb repulsion between o n.n sites;

$$\mathcal{H}^{(5)}_{(i|j),\sigma} = (\lambda_\sigma a_{(i,j),\sigma} - \bar{\lambda}_\sigma a^\dagger_{(i,j),\sigma})[\sum_{\sigma'}(\alpha_{\sigma'}(a^\dagger_{(i\pm1,j),\sigma'} + a^\dagger_{(i,j\pm1),\sigma'}) + \text{h.c.}] \tag{2.67}$$

is the hopping ($t^{(\sigma,\sigma')} \equiv \lambda_\sigma\alpha_{\sigma'}$) and pairing ($p^{(\sigma,\sigma')} \equiv -\lambda_\sigma\alpha^*_{\sigma'}$) between o/• or •/o n.n sites;

$$\mathcal{H}^{(6)}_{(i|j),\sigma} = \underbrace{(\mu_\uparrow\beta_\uparrow - \mu_\downarrow\beta_\downarrow)}_{\equiv \pi}[\,a_{(i\pm1,j)\uparrow}a_{(i\pm1,j)\downarrow} + a_{(i,j\pm1)\uparrow}a_{(i,j\pm1)\downarrow}] + \text{h.c.} \tag{2.68}$$

is the amplitude for the on-site pair formation on o and • sites; and

$$\mathcal{H}^{(7)}_{(i|j),\sigma} = \underbrace{(\mu_\uparrow\beta^*_\uparrow + \mu^*_\downarrow\beta_\downarrow + \beta_\downarrow\beta^*_\uparrow)}_{\equiv t'}(a_{(i\pm1,j),\uparrow}a^\dagger_{(i\pm1,j),\downarrow} + a_{(i,j\pm1),\uparrow}a^\dagger_{(i,j\pm1),\downarrow}) + \text{h.c.} \tag{2.69}$$

is the on-site spin-flip hopping on • sites.

Let us point out some features of the coefficients:

- $\varepsilon_\bullet \neq \varepsilon_\circ$;

- $V^{(\sigma,\sigma')}$ couples both parallel- and antiparallel- spin particles;

- π is zero if both β_σ and μ_σ are independent of σ;

- π and t can be simultaneously eliminated selecting $\varepsilon_0 \equiv 0$.

In case (2), the resulting hamiltonian has, with respect to $H_{(1)}$, two additional contributions and one missing (the Coulomb repulsion $V^{(\sigma,\sigma')}$ between n.n o sites). Thus

$$H_{(2)} = H_{(1)}|_{V=0} + \mathcal{H}^{(8)}_{(i,j),\sigma} + \mathcal{H}^{(9)}_{(i,j),\sigma} \tag{2.70}$$

where

$$\mathcal{H}^{(8)}_{(i|j),\sigma} = \sum_{\sigma'} \underbrace{\left(\alpha_{\sigma'}\beta^*_{-\sigma'} + \alpha^*_{\sigma'}\beta_{-\sigma'}\right)}_{\equiv W} n_{(i,j),\sigma}\left(n_{(i,j\pm1),\sigma'} + n_{(i\pm1,j),\sigma'}\right) \tag{2.71}$$

is the Coulomb repulsion between n.n o/• sites, and

$$\mathcal{H}^{(9)}_{(i|j),\sigma} = \underbrace{\left(\alpha_{\sigma'}\beta^*_{\sigma'} + \alpha^*_{\sigma'}\beta_{\sigma'}\right)}_{\equiv \hat{\tau}} n_{(i,j),\sigma'}\left(a_{(i\pm1,j),\sigma}a^\dagger_{(i\pm1,j),-\sigma} + a_{(i,j\pm1),\sigma}a^\dagger_{(i,j\pm1),-\sigma}\right) + \text{h.c.}$$

$$\tag{2.72}$$

is the on-site hopping at sites • with spin-flip, controlled by the occupancy of the n.n o -sites .

We conclude with the following considerations. First of all, what is really exciting is that the particular form of the superlattice described previously is a direct consequence of the requirement of supersymmetry. Secondly, by cluster mean field one gets, from the above hamiltonian, hamiltonians which are in the same superalgebra as the superlattice Hubbard model, and contains extra terms $A^\dagger_\alpha A_{\bar\alpha}$ and $D_\alpha - N_\alpha$. Thus, diagonalization can be achieved in the standard way. Furthermore, we can expect a thermodynamic phase with two-site order parameters $< a_{\alpha\uparrow}a_{\alpha\downarrow} >$ and $< a_{\alpha\uparrow}a^\dagger_{\alpha\downarrow} >$ and their conjugates both different from zero, even if in the hamiltonian they do not initially appear as it is the case for the pairing operator in the extended Hubbard model.

Moreover, one can infer from the form of $H_{(1)}$ that when such order parameters vanish, then Q could annihilate the vacuum. In other words, a spontaneous summetry breaking would be associated with the appearance of a phase which shows both pairing and magnetic order.

Chapter 3

The extended Falicov-Kimball model

3.1 Introduction

Various generalizations of the Hubbard model have been proposed in order to describe features that the conventional model does not, such as pairing. In particular, in [24] and [25], an additional diagonal term was added, designed to account for Coulomb interaction between nearest neighbour sites. The resulting model is the so-called extended Hubbard model which permits one to treat magnetic and superconducting correlations with a minimum of parameters. The hamiltonian of this model reads

$$
\begin{aligned}
H_{HE} \; = \; & U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{1}{2} V \sum_{<i,j>} \sum_{\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} \\
& + \frac{t}{2} \sum_{<i,j>} \sum_{\sigma,\sigma'} \left(a_{i,\sigma}^\dagger a_{j,\sigma'} + a_{j,\sigma'}^\dagger a_{i,\sigma} \right) \quad .
\end{aligned}
\tag{3.1}
$$

$a_{i,\sigma}^\dagger, a_{i,\sigma}$ are the usual fermionic creation and annihilation over a d-dimensional lattice Λ $(i, j \in \Lambda, \sigma \in \{\uparrow, \downarrow\})$, whereas the parameters U, V, t, have the usual meaning, and $< i, j >$ stands, as customary, for nearest neighbours (n.n.) in Λ.

The model (3.1) can be considered as rather general, resulting from a system of narrow-band electrons strongly coupled to a boson field which they polarize. This field in turn acts onto the electrons thereby forming entirely new quantities described by a correlated motion of the electrons and their surrounding polarization field and by a short-range attraction which can compete with the Coulomb repulsion.

The bosonic modes can be phonons, excitons, acoustic plasmons, etc. The induced attractive potential can partially overcome the Coulomb repulsion and this can give rise to the formation of on-site pairs of electrons if the coupling is strong enough to overcome the usual Hubbard U [3]. For less strong coupling (intermediate-coupling regime) one has essentially intersite pairing due to the short-range effective attraction and on-site as well as long-range Coulomb repulsion [2].

The one-dimensional version has been extensively studied by many people using different methods (renormalization-group techniques, Monte Carlo simulation, exact solution for small clusters, etc.). Despite the apparent simplicity of the extended Hubbard model, there is a rich ground-state phase diagram in terms of the interactions U and V. The ground state of the system can be a spin-density wave (SDW), charge-density wave (CDW), or superconducting state. One important feature of the phase diagram is that there is a SDW-to-CDW transition the line $U = 2V$ for $U > 0$.

In two dimensions, only few numerical results are avalaible but it seems that the situation is qualitatively similar to that in one dimension. In [81], a numerical study of a 4×4 cluster at half-filling is presented, while we refer to [51] for a (Hartree-Fock) mean-field study, where connections with experimental datas about superconductivity and magnetism in La_2CuO_4-based compounds are also presented.

3.2   Linearization and Dynamical Algebra

In the present section we first construct the dynamical algebra of the fermi-linearized version of (3.1) on a dimer. For the sake of simplicity, but with no real loss of generality, we will consider in particular the case in which only one species of electrons (say with up spin) is moving, whereas the other is fixed. This particular version of the Hubbard model has been already studied in the literature [43] and is called the *Falicov-Kimball model* (FK). In the following, we will therefore call our model the extended Falikov-Kimball model.

The FK model has several interesting interpretations; it can be thought of as a model for:

1. a model of crystallization

2. mixed-valence states in rare-earth compounds, where the moving particles play the role of s-band electrons and the localized ones stand for f-electrons with sharp energy level

3. an approximation of the Hubbard model

After relabelling the fermion operators by $A_i \doteq a_{i\uparrow}$, $B_i \doteq a_{i\downarrow}$, $N_i \doteq A_i^\dagger A_i$, and $D_i \doteq B_i^\dagger B_i$, hamiltonian (3.1) can be rewritten (having in mind a grand-canonical ensemble) as

$$
\begin{aligned}
H = & -\mu_A \sum_i N_i - \mu_B \sum_i D_i + \frac{t}{2} \sum_{<i,j>} \left(A_i^\dagger A_j + A_j^\dagger A_i \right) \\
& + U \sum_i N_i D_i + \frac{1}{2} V \sum_{<i,j>} (N_i + D_i)(N_j + D_j) \quad .
\end{aligned}
\tag{3.2}
$$

where μ_A and μ_B are chemical potentials which have to be determined in such a way that the numbers of up and down spins are conserved (as the corresponding operators commute with H). The fact that there is no hopping term between electrons of type B_i has the important consequence that the idempotent number operators D_i commute with each term in (3.2), and can be dealt with as a classical Ising-like variable.

The exact statistical mechanical solution for the FK model is known only for large dimensions [16]. However, a few general theorems are known [43] for the symmetric (or neutral) case $\mu_A = \mu_B = U/2$, and in particular an Ising-like phase transition is expected for dimension $d \geq 2$ at some critical temperature, whose value should vanish both for small and large U. Moreover, there are a number of investigations of the ground state phase diagram in dependence on the configuration of fixed spins [35]. Also a strong-coupling thermodynamic mean-field theory, based on the $d = \infty$ exact solution, was proposed [29].

We proceed now to fermionic linearization over the hopping terms in (3.2). According to the scheme discussed in section(1.2.2), we set

$$
A_i^\dagger A_j \sim \theta_i A_j + A_i^\dagger \bar{\theta}_j - \theta_i \bar{\theta}_j \quad ,
\tag{3.3}
$$

where $\theta_i = < A_i^\dagger >$ ($< \bullet >$ stands for the expectation value of the operator $\bullet$ in some appropriate state (Gibbs or ground)). As usual, $\bar{\theta}, \theta$ are nilpotent variables anticommuting with both the fermion operators $A_i^\dagger, A_i, B_i^\dagger, B_i$ and among themselves.

Furthermore, we perform standard Hartree linearization over the intersite Coulomb interaction terms, *i.e.*

$$
(N_i + D_i)(N_j + D_j) \sim n_0 (N_i + D_i + N_j + D_j) - n_0^2 \quad ,
\tag{3.4}
$$

with $n_0 = < N_i + D_i > = n_A + n_B$.

Both approximations (3.3) and (3.4) will be implemented in the following within the dimer-cluster Fermi-linearization scheme. H reduces thus to an effective hamiltonian denoted here by H_Λ, which is a sum – over an arbitrary set of dimers covering

Λ - of commuting dimer hamiltonians H_d,

$$H_d = \sum_{i=1}^{2} \left[\varepsilon_i N_i + t(q-1)\left(\theta_{\bar{i}} A_i - \bar{\theta}_{\bar{i}} A_i^\dagger\right)\right] + V N_1 N_2 + t\left(A_1^\dagger A_2 + A_2^\dagger A_1\right) + C \quad,$$

(3.5)

where $\varepsilon_i \doteq -\mu_A + U D_{\bar{i}} + V[D_{\bar{i}} + (q-1)n_0]$, and

$$C \doteq \sum_{i=1}^{2} [(-\mu_B + V(q-1)n_0)D_i + t(q-1)\bar{\theta}_i\theta_i] + V\left(D_1 D_2 - (q-1)n_0^2\right) \quad (3.6)$$

is a central term. q denotes the number of nearest neighbours per site in Λ, $\bar{i}$ the site in the dimer which is not i . Furthermore, we assumed that the mean field sensed by site i is the same for each of its neighbours.

H_d as given in (3.5) has a dynamical algebra $\mathcal{A}$ which is the direct sum of 4 copies of a superalgebra $\mathcal{S}$, isomorphic with the Cartan extension by $B_0 \doteq N_1 N_2$ of $su(2|2)$. The latter has a bosonic subalgebra $\mathcal{B}$ isomorphic with $su(2) \oplus su(2)$, generated by the two sets of operators $\{B_1, B_5, B_2\}$ and $\{B_3, B_6, B_4\}$ where

$$B_1 \doteq A_1 A_2 + A_2^\dagger A_1^\dagger \,, B_5 \doteq A_1 A_2 - A_2^\dagger A_1^\dagger \,, B_2 \doteq \mathbb{I} - (N_1 + N_2) \quad, \quad (3.7)$$
$$B_3 \doteq A_1^\dagger A_2 + A_2^\dagger A_1 \,, B_6 \doteq A_1^\dagger A_2 - A_2^\dagger A_1 \,, B_4 \doteq N_1 - N_2 \quad, \quad (3.8)$$

and a fermionic sector $\mathcal{F}$ with eight generators:

$$F_1 = A_1(1 - N_2)\,, F_2 = A_1 N_2\,, F_3 = A_2 N_1\,, F_4 = A_2(1 - N_1) \quad;$$
$$F_{\kappa+4} = F_\kappa^\dagger \quad; \quad \kappa = 1,\ldots,4 \quad. \quad (3.9)$$

B_2 and B_4 are the two Cartan elements of $\mathcal{B}$. Each copy of $\mathcal{S}$ is characterized by a different distribution of the eigenvalues $(0 , 1)$ for the operators D_i entering (3.5).

Let us write the commutation (anticommutation) relations as

$$[\, B_m,\ B_n] = b^p_{mn} B_p \quad, \quad (3.10)$$
$$[\, F_\alpha,\ B_m] = c^\beta_{\alpha m} F_\beta \quad, \quad (3.11)$$
$$\{\tilde{F}_\alpha,\ F_\beta\} = f^m_{\alpha\beta} B_m \quad, \quad (3.12)$$

where $\{b^p_{mn}, c^\beta_{\alpha m}, f^m_{\alpha\beta}\}$ are the structure constants of $\mathcal{S}$.

Due to the fact that only hermitian operators will appear in the hamiltonian, that is $B_1,\ldots,B_4$, in order to simplify further summations over B_i, we have used an unusual numeration of the elements of $\mathcal{B}$.

Now, we can diagonalize the hamiltonian (3.5) by implementing a generalized Bogolubov automorphism in $\mathcal{S}$ rotating H_d into the Cartan sector of $\mathcal{B}$.

3.3 The Diagonalization

3.3.1 The Fermionic Rotation

Since S is a superalgebra, we first act on (3.5) by the adjoint action of a suitable antihermitian rotation operator $\mathcal{Z}_F \in \mathcal{F}$,

$$\mathcal{Z}_F = \sum_{\kappa=1}^{4} (\varphi_\kappa F_\kappa + \bar\varphi_\kappa F_{\kappa+4}) \quad , \tag{3.13}$$

which maps H_d into $H' \doteq \exp(\mathrm{ad}\mathcal{Z}_F)(H_d)$. The coefficients $\varphi_\kappa \in \mathcal{G}_1$ are to be chosen in such a way that H' turns out to be an element of $\mathcal{B}$.

The evaluation of H' for generic φ_ν's gives

$$H' = VB_0 + \sum_{\mu=1}^{4} b_\mu B_\mu + \sum_{\kappa=1}^{4} \left(f_\kappa F_\kappa - \bar f_\kappa F_{\kappa+4} \right) + C' \quad , \quad f_\kappa \in \mathcal{G}_o \quad , \tag{3.14}$$

where, as H' should naturally be hermitian, the operators B_5 and B_6 do not appear: $b_5 = 0$, and $b_6 = 0$.

The coefficients b_μ and f_κ in (3.14) can be expressed in terms of the coefficients $X_\mu^{(m)} \in \mathbb{R}$, and $Y_\nu^{(m)} \in \mathcal{G}_o$, defined by the recursive relation

$$\begin{aligned} (\mathcal{Z}_F)_m \circ H_d &\doteq \left[\mathcal{Z}_F, (\mathcal{Z}_F)_{m-1} \circ H_d \right] \\ &\equiv \sum_{\mu=1}^{4} X_\mu^{(m)} B_\mu + \sum_{\kappa=1}^{4} \left(Y_\kappa^{(m)} F_\kappa - \bar Y_\kappa^{(m)} F_{\kappa+4} \right) \;, \end{aligned} \tag{3.15}$$

with $m \in \mathbb{N}^*$, and $(\mathcal{Z}_F)_0 \circ H_d \equiv H_d$. From the formula

$$\exp(\mathrm{ad}\mathcal{Z}_F) H_d = \sum_{m=0}^{\infty} \frac{1}{m!}((\mathcal{Z}_F)_m \circ H_d), \tag{3.16}$$

it follows that

$$b_\mu = \sum_{m=0}^{\infty} \frac{1}{m!} X_\mu^{(m)} \quad , \quad f_\kappa = \sum_{m=0}^{\infty} \frac{1}{m!} Y_\kappa^{(m)} \quad . \tag{3.17}$$

Let us now deduce the explicit form of the coefficients b_μ's and f_κ's different from zero. For this purpose, we split H_d in two parts,

$$H_d = H_B^{(0)} + H_F^{(0)} \tag{3.18}$$

and we define, for $m \geq 1$

$$H_B^{(m)} = [\mathcal{Z}_F, H_F^{(m-1)}] = X_0^{(m+1)}\mathbb{I} + \sum_{\mu=1}^{4} X_\mu^{(m)} B_\mu \quad , \tag{3.19}$$

$$H_F^{(m)} = [\mathcal{Z}_F, H_B^{(m-1)}] \equiv \sum_{\kappa=1}^{4}(Y_\kappa^{(m)} F_\kappa - \bar{Y}_\kappa^{(m)} F_{\kappa+4}) + \delta_{m,1} V \sum_{i=2}^{3} \varphi_i F_i \tag{3.20}$$

Notice that $H_B^{(0)}$ contains the Cartan extension term VN_1N_2 giving rise in $H_F^{(1)}$ to the extra term explicitly written in $H_F^{(m)}$. It follows that

$$
\begin{aligned}
H_B^{(m+1)} &= \sum_{\alpha,\kappa=1}^{4} \left(-\phi_\alpha Y_\kappa^{(m)}\{F_\alpha, F_\kappa\} + \phi_\alpha \bar{Y}_\kappa^{(m)}\{F_\alpha, F_{\kappa+4}\} \right) + \text{h.c} \\
&= X_0^{(m+1)}\mathbb{I} + \sum_{\mu=1}^{4} \underbrace{\left(\left(-\phi_\alpha f_{\alpha\kappa}^\mu Y_\kappa^{(m)} + \phi_\alpha f_{\alpha,\kappa+4}^\mu \bar{Y}_\kappa^{(m)}\right) + \text{h.c.} \right)}_{X_\mu^{(m+1)}} B_\mu \quad (3.21)
\end{aligned}
$$

$$
\begin{aligned}
H_F^{(m+1)} &= \sum_{\mu=1}^{4} X_\mu^{(m)} \sum_{\alpha=1}^{4} \left(\phi_\alpha[F_\alpha, B_\mu] + \bar{\phi}_\alpha[F_{\alpha+4}, B_\mu] \right) \\
&= \sum_{\kappa=1}^{4} \underbrace{\left(\sum_{\mu=1}^{4} X_\mu^{(m)} \sum_{\alpha=1}^{4} c_{\alpha\mu}^\kappa \phi_\alpha \right)}_{Y_\kappa^{(m+1)}} F_\kappa + \text{h.c.} \quad . \tag{3.22}
\end{aligned}
$$

The commutators (3.21) and (3.22) lead to the definition of two matrices transfering fermionic coefficients to bosonic and viceversa, at each step. The more convenient way to solve the problem is to restrict the action of this transfer matrices to the set of coefficients $\{X_\mu^{(m)}, Y_\kappa^{(m)} ; \mu, \kappa = 1, \ldots, 4\}$. Namely, the operator B_0 appears only in $H_B^{(0)}$ while the contributions to the constant term arising from the commutators $[\mathcal{Z}_F, H_F^{(m)}]$, $m \geq 0$ will be calculated separately.

After this preliminary statement, we define the kets $\mid X^{(m)} >$ and $\mid Y^{(m)} >$ denoting 4-vectors whose components are labelled by $\mu, \kappa = 1, \ldots, 4$ and the "reduced" 4×4-matrices $\mathbf{R}, \mathbf{S}$ calculated from (3.21) and (3.22):

$$
\mathbf{R} = \begin{pmatrix} -\varphi_3 & \varphi_4 & -\varphi_1 & \varphi_2 \\ -\bar{\varphi}_1 & \bar{\varphi}_2 & \bar{\varphi}_3 & -\bar{\varphi}_4 \\ -\bar{\varphi}_4 & \bar{\varphi}_3 & \bar{\varphi}_2 & -\bar{\varphi}_1 \\ -\bar{\varphi}_1 & \bar{\varphi}_2 & -\bar{\varphi}_3 & \bar{\varphi}_4 \end{pmatrix} \quad , \quad \mathbf{S} = \begin{pmatrix} -\bar{\varphi}_3 & -\varphi_1 & \varphi_4 & \varphi_1 \\ -\bar{\varphi}_4 & -\varphi_2 & \varphi_3 & \varphi_2 \\ \bar{\varphi}_1 & -\varphi_3 & \varphi_2 & -\varphi_3 \\ \bar{\varphi}_2 & -\varphi_4 & \varphi_1 & -\varphi_4 \end{pmatrix} \quad , \tag{3.23}
$$

such that $\mid Y^{(m+1)} >= \mathbf{S} \mid X^{(m)} >$, $\mid X^{(m+1)} >= \mathbf{R} \mid Y^{(m)} >$. Gluing together the last two relations, the following recursive relation holds as well:

$$\mid X^{(m+2)} >= \mathbf{P} \mid X^{(m)} > \quad , \quad \mathbf{P} = \mathbf{RS} \quad . \tag{3.24}$$

$\mathbf{P}$ is a 4×4 matrix whose elements ($\in \mathcal{G}_e$) are given by

$$\mathbf{P} = \begin{pmatrix} a & 0 & b & c \\ 0 & a & d & e \\ -b & -d & -a & 0 \\ -c & -e & 0 & -a \end{pmatrix} \quad , \tag{3.25}$$

where

$$\begin{aligned} a &= -\varphi_1\bar{\varphi}_1 + \varphi_2\bar{\varphi}_2 + \varphi_3\bar{\varphi}_3 - \varphi_4\bar{\varphi}_4 \quad , \\ b &= -2(\varphi_1\varphi_2 + \varphi_3\varphi_4) \quad , \\ c &= 2(\varphi_1\varphi_3 - \varphi_2\varphi_4) \quad , \\ d &= 2(\varphi_1\varphi_4 - \varphi_2\varphi_3) \quad , \\ e &= \varphi_1\bar{\varphi}_1 - \varphi_2\bar{\varphi}_2 + \varphi_3\bar{\varphi}_3 - \varphi_4\bar{\varphi}_4 \quad . \end{aligned} \tag{3.26}$$

Defining

$$\begin{aligned} \alpha_1 &= b^2 + c^2 & \alpha_2 &= b^2 + d^2 \\ \beta_1 &= bd + ce & \beta_2 &= bc + de \\ \gamma_1 &= d^2 + e^2 & \gamma_2 &= c^2 + e^2 \end{aligned} \tag{3.27}$$

and

$$\mathbf{A}_i = \begin{pmatrix} a^2 - \alpha_i & -\beta_i \\ -\beta_i & a^2 - \gamma_i \end{pmatrix} \quad , \quad \Omega_i = \begin{pmatrix} \lambda_+^{(i)} & 0 \\ 0 & \lambda_-^{(i)} \end{pmatrix} \tag{3.28}$$

we can write $\mathbf{P}^2 = \mathbf{A}_1 \oplus \mathbf{A}_2$. The eigenvalues and the eigenvectors of $\mathbf{P}^2$ are then given by

$$z_\alpha^i = \lambda_{(-)^{(\alpha+1)}}^{\left(\left[\frac{\alpha+1}{2}\right]\right)} \quad , \quad \alpha = 1,\dots,4 \quad , \tag{3.29}$$

$$v_\pm^i = \begin{pmatrix} \beta_i \\ \frac{1}{2}(\gamma_i - \alpha_i \mp \sqrt{\Delta_i}) \end{pmatrix} \tag{3.30}$$

where

$$\lambda_\pm^{(i)} = \frac{1}{2}(2a^2 - \alpha_i - \gamma_i \pm \sqrt{\Delta_i}), \quad \Delta_i = (\alpha_i - \gamma_i)^2 + 4\beta_i^2. \tag{3.31}$$

Defining the 2×2 matrices $\mathbf{R}_i = (v_+^i, v_-^i)$, $i = 1,2$, the rotation matrix $\mathbf{T}$ diagonalizing $\mathbf{P}^2$ can be written as $\mathbf{T} = \mathbf{R}_1 \oplus \mathbf{R}_2$. With $\Omega = \Omega_1 \oplus \Omega_2$ we have therefore $\mathbf{P}^2 = \mathbf{T}\,\Omega\,\mathbf{T}^{-1}$.

As the matrix $\mathbf{P}^2$ turns out to be block diagonal (two 2×2 blocks), it is convenient to express the first of equations (3.17), upon implementing (3.24), as a series of even powers of $\mathbf{P}$, assuming the first four $|X^{(m)}>$'s, namely $m = 0 \ldots, 3$, as primitive. For the kets $| b >$ and $| f >$, we therefore obtain

$$| b > = \sum_{l=0}^{3} \sum_{k=0}^{\infty} \frac{\mathbf{P}^{2k}}{(4k + l)!} | X^{(l)} > \quad , \qquad (3.32)$$

$$| f > = | Y^{(0)} > + | \Gamma > + \sum_{l=1}^{4} \sum_{k=0}^{\infty} \mathbf{S} \frac{\mathbf{P}^{2k}}{(4k + l)!} | X^{(l-1)} > \qquad (3.33)$$

where $Y_1^{(0)} = Y_2^{(0)} \doteq \tau \theta_1$, $Y_3^{(0)} = Y_4^{(0)} \doteq \tau \theta_2$, and $\Gamma_\nu \in \mathcal{G}_1$ are the coefficients of the fermionic operators obtained by the commutation of $\mathscr{Z}_F$ with the operator $N_1 N_2$.

Setting $\kappa_{\mu,\mu'}^{(\alpha)} = (\mathbf{T}^{-1})_{\mu,\alpha}(\mathbf{T})_{\alpha,\mu'}$, one finally obtains the b_μ's in (3.32) as

$$b_\mu = \sum_{\mu'=1}^{4} \sum_{\ell=0}^{3} \mathcal{L}_{\mu,\mu'}^{(\ell)} X_{\mu'}^{(\ell)} \quad , \qquad (3.34)$$

with

$$\mathcal{L}_{\mu,\mu'}^{(\ell)} = \sum_{\alpha=1}^{4} \kappa_{\mu,\mu'}^{(\alpha)} z_\alpha^{-\ell} \frac{d^{4-\ell} \mathscr{Z}_\alpha}{d z_\alpha^{4-\ell}}, \qquad (3.35)$$

$$\mathscr{Z}_\alpha = \left(\cosh(z_\alpha) + \cos(z_\alpha)\right)\Theta(z_\alpha) - \cosh(\frac{z_\alpha}{\sqrt{2}})\cos(\frac{z_\alpha}{\sqrt{2}})\Theta(-z_\alpha),$$

where $\Theta(x)$ is the usual Heaviside step-function: $\Theta(x) = 0$ when $x < 0$ and $\Theta(x) = 1$ when $x \geq 0$. For the coefficients of (3.33), one also obtains in analogous way

$$f_\nu = Y_\nu^{(0)} + \Gamma_\nu + \sum_{\mu=1}^{4} S_{\nu,\mu} \mathcal{T}_\mu \quad , \qquad (3.36)$$

where

$$\mathcal{T}_\mu = \sum_{\mu'=1}^{4} \sum_{\ell=1}^{4} \left(\mathcal{L}_{\mu,\mu'}^{(\ell)} X_{\mu'}^{(\ell-1)} - X_{\mu'}^{(2)} \kappa_{\mu,\mu'}^{(\ell)} z_\ell^{-4} \right) \quad . \qquad (3.37)$$

As for the term proportional to the identity, upon defining the vector $| q >$ as

$$| q > = \begin{pmatrix} -2(\varphi_1 \varphi_3 + \varphi_2 \varphi_4) \\ -(\varphi_1 \bar{\varphi}_1 + \varphi_2 \bar{\varphi}_2 + \varphi_3 \bar{\varphi}_3 + \varphi_4 \bar{\varphi}_4) \\ 2(\varphi_1 \bar{\varphi}_4 + \varphi_2 \bar{\varphi}_3) \\ \varphi_1 \bar{\varphi}_1 + \varphi_2 \bar{\varphi}_2 - \varphi_3 \bar{\varphi}_3 - \varphi_4 \bar{\varphi}_4 \end{pmatrix}, \qquad (3.38)$$

we obtain

$$\mathcal{C}' = \mathcal{C} + \sum_{\alpha=1}^{4}(Y_{\alpha}^{(0)}\bar{\varphi}_{\alpha}) + \frac{1}{2}V(\varphi_2\bar{\varphi}_2 - \varphi_3\bar{\varphi}_3)$$
$$+ \sum_{\alpha=1}^{4} q_{\alpha} \sum_{\gamma,l=1}^{4} \left(\mathcal{L}_{\alpha\gamma}^{(l+1)} b_{\gamma}^{(l-1)} - \kappa_{\alpha\gamma}^{(l)} z_l^{-4}(b_{\gamma}^{(2)} + b_{\gamma}^{(3)}) \right). \tag{3.39}$$

H' as given by (3.14) is an element of $\mathcal{B}$, if the coefficients f_{ν} given by (3.36) equal zero. The latter requirement gives rise to a system of four equations in the unknown $\varphi_{\nu} \in \mathcal{G}_1$. In order to solve it, it is convenient to express both the θ's and the φ's as linear combinations with coefficients in $\mathbb{R}$ of two anticommuting units ξ and $\bar{\xi} \in \mathcal{G}_1$, with $\xi\bar{\xi} = 1$. More precisely we choose

$$\theta_i = \rho_i\xi + \sigma_i\bar{\xi} \quad , \quad \varphi_{\nu} = r_{\nu}\xi + s_{\nu}\bar{\xi} \quad . \tag{3.40}$$

Once the above representation has been inserted in the system (3.36) and the equation (3.37), by separately setting equal to zero the coefficients of the ξ and the $\bar{\xi}$ part of each equation, one finally gets a system of eight equations in the real unknown r_{ν} and s_{ν} ($\nu = 1,\ldots,4$). This system explicitly reads

$$\begin{cases} -s_3\mathcal{T}_1 - r_1\mathcal{T}_2 + r_4\mathcal{T}_3 + r_1\mathcal{T}_4 = -\tau\rho_1 \\ -s_4\mathcal{T}_1 - r_2\mathcal{T}_2 + r_3\mathcal{T}_3 + r_2\mathcal{T}_4 = -\tau\rho_1 - Vr_2 \\ s_1\mathcal{T}_1 - r_3\mathcal{T}_2 + r_2\mathcal{T}_3 - r_3\mathcal{T}_4 = -\tau\rho_2 - Vr_3 \\ s_2\mathcal{T}_1 - r_4\mathcal{T}_2 + r_1\mathcal{T}_3 - r_4\mathcal{T}_4 = -\tau\rho_2 \end{cases} \tag{3.41}$$

$$\begin{cases} -r_3\mathcal{T}_1 - s_1\mathcal{T}_2 + s_4\mathcal{T}_3 + s_1\mathcal{T}_4 = -\tau\sigma_1 \\ -r_4\mathcal{T}_1 - s_2\mathcal{T}_2 + s_3\mathcal{T}_3 + s_2\mathcal{T}_4 = -\tau\sigma_1 - Vs_2 \\ r_1\mathcal{T}_1 - s_3\mathcal{T}_2 + s_2\mathcal{T}_3 - s_3\mathcal{T}_4 = -\tau\sigma_2 - Vs_3 \\ r_2\mathcal{T}_1 - s_4\mathcal{T}_2 + s_1\mathcal{T}_3 - s_4\mathcal{T}_4 = -\tau\sigma_2 \end{cases} \tag{3.42}$$

One then solves, say, the first system in the variables $\mathcal{T} = \mathcal{T}(r_{\alpha}, s_{\alpha})$ and substitutes them in the second. This new system, due to the complicate form of the $\mathcal{T}$ is highly non-linear in the variables r_{α} and s_{α} and must be solved numerically.

We shall denote their solution by $\{\tilde{r}_{\nu}, \tilde{s}_{\nu}\}$, and by $\tilde{b}_{\mu}$ the expressions (3.34) evaluated at $r_{\nu} = \tilde{r}_{\nu}$, $s_{\nu} = \tilde{s}_{\nu}$. We also denote as $\tilde{H}'$ the rotated bosonic hamiltonian given now by

$$\tilde{H}' = VB_0 + \sum_{\mu=1}^{4} \tilde{b}_{\mu}B_{\mu} + \tilde{\mathcal{C}}' \quad . \tag{3.43}$$

It is worth noticing how $\tilde{H}'$ contains the off-diagonal pairing operator B_1, even though H_d doesn't. As mentioned in section(2.8), this makes the model considered

particularly interesting in view of high T_c superconductivity, as such operators were intrinsically generated by the dynamical algebra of the system, and may therefore be expected to give rise to non-vanishing order parameters.

3.3.2 The case $D_1 = D_2$

For two of the four copies of S, when the eigenvalues of the operators D_1, D_2 are equal, the equations for the rotation parameters φ_ν can be solved exactly. This is due to the fact that in equation (3.5), we obtain $\varepsilon_1 = \varepsilon_2 \equiv \bar{\varepsilon}$ and we can set $\theta = \theta_1 = \theta_2$ because of the exchange symmetry between the two dimer sites. Defining

$$\left. \begin{array}{l} \bar{\varepsilon}_{(0,0)} = \varepsilon + W \\ C_{(0,0)} = 2\kappa + \varepsilon + W \end{array} \right\} \; D_1 = D_2 = 0 \tag{3.44}$$

and

$$\left. \begin{array}{l} \bar{\varepsilon}_{(1,1)} = \varepsilon + U + V + W \\ C_{(1,1)} = 3(\varepsilon + W) + 2(\kappa + V) + U \end{array} \right\} \; D_1 = D_2 = 1 \tag{3.45}$$

where

$$W := V(q-1)n_0 \quad ; \quad \kappa := (t\bar{\theta}\theta + \frac{V}{2}n_0^2)(q-1) \quad , \tag{3.46}$$

we obtain

$$H_d^{(i)} := -\bar{\varepsilon}_{(i,i)}B_2 + tB_3 + VN_1N_2 + \tau\sum_{i=1}^{4}(\theta F_i - \bar{\theta}F_{i+4}) + C_{(i,i)} \quad . \tag{3.47}$$

$\mathscr{Z}_F$ in equation (3.13) becomes

$$\mathscr{Z}_F = \varphi_1(F_1 + F_4) + \varphi_2(F_2 + F_3) - \text{h.c} \tag{3.48}$$

and

$$\exp(\text{ad}\mathscr{Z}_F)(H_d^{(i)}) = H_d^{(i)} + [\ \mathscr{Z}_F \ , \ H_d^{(i)}] + \frac{1}{2}[\ \mathscr{Z}_F, \ [\mathscr{Z}_F \ , \ H_d^{(i)}]\ ] \quad , \tag{3.49}$$

because commutators of higher order in (3.16) vanish.

It is worth noticing that only two angles φ_1, φ_2 are sufficient to cancel the fermionic part since the dynamical algebra of $H_d^{(i)}$ is in fact a subalgebra of S generated by the eight operators $\{\ B_0, \ B_2, \ B_3, \ \mathbb{I}\ ; \ F_1+F_4, \ F_2+F_3, \ F_5+F_8, \ F_6+F_7\}$. A simple calculation leads to the solution

$$\tilde{\varphi}_1 = -\frac{\tau\theta}{\bar{\varepsilon}+t} \quad , \quad \tilde{\varphi}_2 = -\frac{\tau\theta}{V+\bar{\varepsilon}+t} \quad , \tag{3.50}$$

and the coefficients for the hamiltonian (3.43) are in this case

$$
\begin{aligned}
\tilde{b}_2 &= -(\tilde{\varepsilon} + V_R \tau^2 \theta \bar{\theta}) \quad , \\
\tilde{b}_3 &= t - V_R \tau^2 \theta \bar{\theta} \quad , \\
\tilde{C}' &= C - \tau^2 \theta \bar{\theta}(V_R + \frac{2}{V + \tilde{\varepsilon} + t})
\end{aligned}
\tag{3.51}
$$

where

$$
V_R := \frac{V}{(\tilde{\varepsilon} + t)(V + \tilde{\varepsilon} + t)}
\tag{3.52}
$$

and the indices (i, i) denoting the projection are omitted.

3.3.3 The bosonic rotation

We can now proceed to the rotation of $\tilde{H}'$ into H'', by means of the adjoint action of $\mathcal{Z}_B = z\, B_5 + w\, B_6 \in \mathcal{B}$; $z, w \in \mathbb{R}$. Of course, as the rotation is an automorphism in $\mathcal{B}$, H'' will still be of the form

$$
H'' = V B_0 + \sum_{\mu=1}^{4} h_\mu B_\mu + \tilde{C}' \quad .
\tag{3.53}
$$

Let us define $\tilde{H}'^{(m+1)} = [\, \mathcal{Z}_B,\ \tilde{H}'^{(m)}\,]\,, m \geq 0$. Then $\mid \tilde{b}^{(m)} >= \Omega^m \mid \tilde{b} >$, with

$$
\Omega = \begin{pmatrix}
0 & -2z & 0 & 0 & z \\
2z & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -2w & 0 \\
0 & 0 & 2w & 0 & 0 \\
z & 0 & 0 & 0 & 0
\end{pmatrix} \quad .
\tag{3.54}
$$

and from $\mid h >= \exp(\Omega)\mid \tilde{b} >$, the exponentiation of the matrix Ω leads to

$$
\begin{aligned}
h_1 &= \tilde{b}_1 \cos 2w + (\frac{V}{2} - \tilde{b}_2) \sin 2w \quad , \\
h_2 &= (\tilde{b}_2 - \frac{V}{2}) \cos 2w + \tilde{b}_1 \sin 2w + \frac{1}{2}V \quad , \\
h_3 &= \tilde{b}_3 \cos 2z - \tilde{b}_4 \sin 2z \quad , \\
h_4 &= \tilde{b}_4 \cos 2z + \tilde{b}_3 \sin 2z \quad .
\end{aligned}
\tag{3.55}
$$

In order for $\mathcal{H}$ to be diagonal, the equations $h_1 = 0 = h_3$ must be satisfied. These can be easily solved in z, w. Denoting the solution by $\tilde{z}, \tilde{w}$, one has

$$
\tilde{w} = \frac{1}{2}\arctan\left(\frac{2\tilde{b}_1}{2\tilde{b}_3 - V}\right) \quad , \quad \tilde{z} = \frac{1}{2}\arctan\left(\frac{\tilde{b}_3}{\tilde{b}_4}\right) \quad .
\tag{3.56}
$$

With the above choices $\mathcal{H}$ finally reads

$$\mathcal{H} = (\tilde{h}_4 - \tilde{h}_2)N_1 - (\tilde{h}_4 + \tilde{h}_2)N_2 + VN_1N_2 + C'' \quad , \tag{3.57}$$

where

$$
\begin{aligned}
\tilde{h}_2 &= \sqrt{\tilde{b}_1^2 + (\tilde{b}_2 - \frac{V}{2})^2} + \frac{V}{2} \quad , \\
\tilde{h}_4 &= \sqrt{\tilde{b}_3^2 + \tilde{b}_4^2} \quad , \\
C'' &= \bar{C}' + \tilde{h}_2 \quad .
\end{aligned}
\tag{3.58}
$$

Of course, the spectrum is given by (3.57) setting $N_i = 0, 1$ for $i = 1, 2$.

3.4 Partition function and self-consistency equations

The spectrum of hamiltonian (3.57) still depends (through $\tilde{h}_2$, $\tilde{h}_4$) on a set of classical Ising-like configuration variables, *i.e.* the D_i's. The expectation value of the latter cannot evolve dynamically under the action of the linearized hamiltonian (3.5), since their commutator with it (as well as with (3.2)) vanishes. Nevertheless, since we aim to know which is the configuration of the D_i's most favourable from the point of view of the free energy, in the frame of a dimer approximation, we should average over the distribution of the D_i's in Λ. We do this by summing within the partition function Z over all possible configurations of the D_i's in the dimer, having introduced a chemical potential μ_B fixing their average number (specified by the magnetization m). In other words, we let μ_B incorporate all necessary information on the distribution of the D_i's over the lattice with a weight which is a Gibbs probability. Explicitly

$$
\begin{aligned}
Z &\doteq \sum_{D_1,D_2=0,1} \sum_{N_1,N_2=0,1} \exp -\beta\mathcal{H} \\
&= e^{-\beta C''} \left[1 + e^{\beta \tilde{h}_2} \left(2\cosh\beta\tilde{h}_4 + e^{\beta(\tilde{h}_2 - V)} \right) \right] \quad .
\end{aligned}
\tag{3.59}
$$

In order to obtain quantitative predictions from equation (3.59), we must first evaluate the variables θ_i as well as the filling n_0 consistently with their definitions (3.3) and (3.4). Moreover, the magnetization $m \doteq < N_i - D_i > = n_A - n_B$ has to be fixed. This requires to compute the expectation values $< A_i^\dagger >$ and $< N_i \pm D_i >$ respectively. This is straightforwardly achieved upon recalling that, for any operator $\Omega \in \mathcal{A}$ (different from B_0), we have

$$
\begin{aligned}
< \Omega > &= \frac{1}{Z} \mathrm{Tr} \left[\Omega \, e^{-\beta H_d} \right] \\
&= \frac{1}{Z} \mathrm{Tr} \left\{ \exp(\mathrm{ad}\tilde{Z}_B)(\exp(\mathrm{ad}\tilde{Z}_F)(\Omega)) \, e^{-\beta\mathcal{H}} \right\} \quad ,
\end{aligned}
\tag{3.60}
$$

where $\tilde{Z}_B$ and $\tilde{Z}_F$ are of course those antihermitian rotation operators which diagonalize H_d.

Upon denoting by Ω' the rotated operator $\exp(\text{ad}\tilde{Z}_F)(\Omega)$, we observe that Ω' is given by a formula completely analogous to (3.14) (with $V = 0$), in which one has to replace the b_μ's, f_κ's and C' by $b_\mu^{(\Omega)}$'s, $f_\kappa^{(\Omega)}$'s and C'_Ω. The latter are still expressed by equations (3.17) to (3.39), in which only the initial vectors $\mid X^{(\ell)} > (\ell = 0, 1, 2, 3)$ and $\mid Y^{(0)} >$ have been replaced by $\mid X^{(\ell)} >^\Omega$ and $\mid Y^{(0)} >^\Omega$, and are obtained by (3.15) upon substituting H_d with Ω.

Also, when evaluating $\Omega'' \doteq \exp(\text{ad}\tilde{Z}_B)(\Omega')$ in (3.60), we can disregard the contribution of the fermionic operators in Ω', as they remain fermionic after bosonic rotation, and hence have vanishing expectation value in the basis in which $\mathcal{H}$ is diagonal. This implies that formula (3.57)-(3.58) hold even for Ω'' (once more setting $V = 0$), where of course the appropriate $b_\mu^{(\Omega)}$'s (same expression as in (3.34) with $|X^{(\ell)} >^\Omega$ instead of $|X^{(\ell)} >$) have to be used instead of $\tilde{b}_\mu$'s in the definition of the corresponding $h_\mu^{(\Omega)}$'s. Recalling again that only the operators diagonal in the Cartan basis contribute to the trace in (3.60), we finally get

$$< \Omega > = \frac{1}{Z} \sum_{\{D_i\}} \sum_{\{N_j\}} (h_2^{(\Omega)}(\{D_i\})(1 - N_1 - N_2) + h_4^{(\Omega)}(\{D_i\})(N_1 - N_2)$$
$$+ C^{(\Omega)}(\{D_i\})) \, e^{-\beta\mathcal{H}(\{D_i\},\{N_j\})} \quad , \tag{3.61}$$

with

$$h_2^{(\Omega)} = b_1^{(\Omega)} \sin 2\tilde{w} + b_2^{(\Omega)} \cos 2\tilde{w} \quad , \quad h_4^{(\Omega)} = b_3^{(\Omega)} \sin 2\tilde{z} + b_4^{(\Omega)} \cos 2\tilde{z} \quad . \tag{3.62}$$

Applying (3.61) successively with $\Omega = \frac{1}{2}(\theta_1 A_1 - \bar{\theta}_1 A_1^\dagger), \frac{1}{2}(\theta_2 A_2 - \bar{\theta}_2 A_2^\dagger), \frac{1}{2}\{N_1 + N_2 \pm (D_1 + D_2)\}$, we obtain the four consistency equations to be satisfied, by setting at the *l.h.s.* of (3.61) $\theta_1\bar{\theta}_1$, $\theta_2\bar{\theta}_2$, n_0 and m respectively. The latter equations of course are to be solved in the four unknowns $\theta_1\bar{\theta}_1$, $\theta_2\bar{\theta}_2$, μ_A and μ_B. While the first three of these equations are in general highly non-linear, the fourth can be solved rigorously. Defining $p = < D_i >= (n_0 - m)$, we obtain μ_B as a function of the other unknowns:

$$\exp \beta\mu_B = \frac{1}{(p-2)Y_2} \left\{ Y_1(1 - p) + \sqrt{(p-1)^2 Y_1^2 - p(p-2)Y_0 Y_2} \right\} \quad , \tag{3.63}$$

where

$$Y_\kappa \doteq \mathcal{H}|_{D_1 + D_2 = \kappa} + \kappa\mu_B \quad , \quad \kappa = 0, 1, 2 \quad , \tag{3.64}$$

is in fact independent of μ_B.

Obviously, any expectation value of operators in S can be evaluated by means of (3.61)-(3.62), once the vectors $\mid X^{(\ell)} >^{\Omega}$ and $\mid Y^{(0)} >^{\Omega}$ have been specified.

In particular, for the pairing operator B_1 we have

$$
\mid X^{(0)} >^{B_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad , \quad \mid X^{(2)} >^{B_1} = \begin{pmatrix} a \\ 0 \\ -b \\ -c \end{pmatrix} ,
$$

$$
\mid X^{(1)} >^{B_1} = \mid X^{(3)} >^{B_1} = \mid Y^{(0)} >^{B_1} = 0 \quad , \tag{3.65}
$$

with a, b and c defined in formulas (3.26). It is important noticing that, depending on the physical parameters U, t, and V, the expression (3.60) implemented with $\Omega \equiv B_1$, together with (3.65), give a non-vanishing expectation value for the pairing operator. On the contrary, when $V = 0$ the latter turns out to be identically zero.

The last observation suggests once more that the intersite Coulomb repulsion could play a possible role in the onset of superconductivity. Hence, a more detailed analysis of the ground state behavior, as well as of the thermodynamical properties of our approximation to the model, are expected to give interesting results.

Nevertheless, because of the great number of equations (in principle there are nineteen ones) which have to be satisfied in order to guarantee both the self-consisten cy constraints and the requirements on the coefficients of the Bogolubov rotations are properly implemented, their solutions is a very delicate numerical problem. Hence, in order to gain a more detailed description of the phase space, one should first consider solutions with special symmetries and this will be done in the next section.

3.5 The homogeneous solution.

We now turn to the detailed discussion of the homogeneous case, which consists in setting $\theta_1 = \theta = \theta_2$. Such a choice leads, due to the Grassmann-like nature of the variable θ, to zero expectation value for the pairing. [1]

Even though this makes the solution slighltly less general from the physical point of view, it leads to a much better insight into the equations structure.

---

[1] *It is straightforward to check that the system for the rotation parameters has in this case the solution $s_1 = s_2 = s_3 = s_4 = 0$, i.e. $\varphi_\kappa \propto \theta$. This implies that the fermionic rotation on the one hand does not generate a pairing operator in the hamiltonian H', therefore, as $\tilde{b}_1 = 0$, one gets $\tilde{w} = 0$. On the other hand B_1' turns out to be proportional to B_1, $(b_1^{(B_1)} \neq 0, b_j^{(B_1)} = 0$ for $j = 2, 3, 4)$, hence $h_2^{(B_1)} = h_4^{(B_1)} = 0$, and, since also $C^{(B_1)} = 0$, finally $< B_1 >= 0$.*

With the above choice the hamiltonian reads

$$H = \varepsilon_1 N_1 + \varepsilon_2 N_2 + t(A_1^\dagger A_2 + A_2^\dagger A_1) + V N_1 N_2$$
$$\tau(\theta A_1 - \bar\theta A_1^\dagger + \theta A_2 - \bar\theta A_2^\dagger) + C \tag{3.66}$$

where $\tau = t(q - 1)$. Instead of applying the general scheme for the diagonalization sketched in the previous paragraph, in this case it is more convenient to implement the rotation of H in five successive steps, by acting on it with the adjoint action of the following five (three bosonic and two fermionic) antihermitian operators

$$Z_B^{(i)} = p_i(A_1^\dagger A_2 - A_2^\dagger A_1), \quad i = 1, 2, 3 \tag{3.67}$$

$$Z_F^{(1)} = \mu(1 - N_2)(\theta A_1 + \bar\theta A_1^\dagger) + \nu(1 - N_1)(\theta A_2 + \bar\theta A_2^\dagger), \tag{3.68}$$

$$Z_F^{(2)} = \rho N_2(\theta A_1 + \bar\theta A_1^\dagger) + \sigma N_1(\theta A_2 + \bar\theta A_2^\dagger)$$
$$= \rho(\theta F_2 + \bar\theta F_6) + \sigma(\theta F_3 + \bar\theta F_7). \tag{3.69}$$

Thus, the number of non-linear equations for the rotation parameters which diagonalizes H reduces now to four.

Indeed, by applying successively $Z_B^{(1)}, Z_F^{(1)}, Z_B^{(2)}$, with an appropriate choice of the parameters $\{p_1, p_2, \mu, \nu\}$, we can project the fermionic operators into the $\mathcal{F}$-subset $\{F_2, F_3, F_6, F_7\}$. Choosing $p_1 = \dfrac{1}{2}\tan^{-1}\dfrac{2t}{\varepsilon_1 - \varepsilon_2}$, we obtain

$$H^{(1)} = \varepsilon_+ N_1 + \varepsilon_- N_2 + + V N_1 N_2 + \tau(\alpha_+(\theta A_1 - \bar\theta A_1^\dagger) + \alpha_-(\theta A_2 - \bar\theta A_2^\dagger)) + C \tag{3.70}$$

where

$$\varepsilon_\pm = \frac{1}{2}(\varepsilon_1 + \varepsilon_2 \pm \eta\sqrt{\Delta}), \quad \eta = sgn(\varepsilon_1 - \varepsilon_2)$$

$$\Delta = (\varepsilon_1 - \varepsilon_2)^2 + 4t^2 \tag{3.71}$$

$$\alpha_\pm = \cos p_1 \pm \sin p_1 \quad . \tag{3.72}$$

Then, with $\mu = -\dfrac{\tau\alpha_+}{\varepsilon_+}, \nu = -\dfrac{\tau\alpha_-}{\varepsilon_-}$ in $Z_F^{(1)}$, we eliminate the operators F_1, F_4, F_5, F_8 and it results

$$H^{(2)} = \varepsilon_+' N_1 + \varepsilon_-' N_2 + V N_1 N_2 + t''(A_1^\dagger A_2 + A_2^\dagger A_1)$$
$$+ V(\mu N_2(\theta A_1 - \bar\theta A_1^\dagger) + \nu N_1(\theta A_2 - \bar\theta A_2^\dagger)) + C \tag{3.73}$$

where

$$\varepsilon_+' = \varepsilon_+ - 2V\bar\theta\theta\nu^2$$

$$\varepsilon_+' = \varepsilon_- - 2V\bar\theta\theta\mu^2 \tag{3.74}$$

$$t'' = \frac{2\tau^2 V\bar\theta\theta}{\varepsilon_+\varepsilon_-}\cos 2p_1$$

Finally, we can eliminate one more time the pairing operator, choosing $\tan 2p_2 = \dfrac{2t''}{\varepsilon'_+ - \varepsilon'_-}$ in $Z_B^{(2)}$ obtaining therefore:

$$
\begin{aligned}
H^{(3)} &= \exp(\mathrm{ad} Z_B^{(2)}) \exp(\mathrm{ad} Z_F^{(1)}) \exp(\mathrm{ad} Z_B^{(1)})\, H \\
&= \varepsilon'_1 N_1 + \varepsilon'_2 N_2 + V N_1 N_2 + C + V(\gamma(\theta F_2 - \bar{\theta} F_6) + \delta(\theta F_3 - \bar{\theta} F_7))
\end{aligned}
\tag{3.75}
$$

with

$$
\begin{aligned}
\varepsilon'_1 &= \tfrac{1}{2}(\varepsilon'_+ + \varepsilon'_- + \eta'\sqrt{\Delta'}) \quad,\quad \eta' = sgn(\varepsilon'_+ - \varepsilon'_-) \\
\varepsilon'_2 &= \tfrac{1}{2}(\varepsilon'_+ + \varepsilon'_- - \eta'\sqrt{\Delta'}) \\
\Delta' &= (\varepsilon'_+ - \varepsilon'_-)^2 + 4t''^2 \\
\gamma &= \mu \cos p_2 + \nu \sin p_2 \\
\delta &= \nu \cos p_2 - \mu \sin p_2.
\end{aligned}
\tag{3.76}
$$

$$
\tag{3.77}
$$

In order to cancel the fermionic part of (3.75), we act on it applying $Z_F^{(2)}$. This gives

$$
H^{(4)} = b_1 N_1 + b_2 N_2 + b_3 B_3 + b_4 N_1 N_2 + \sum_{k=1}^{2} f_k(\theta F_{k+1} - \bar{\theta} F_{k+5}) + C \quad,
\tag{3.78}
$$

where $b_i, f_j \in \mathbb{R}$, $(i = 1, \ldots, 4; j = 1, 2)$. As before we denote by $b_i^{(m)}$ and $f_i^{(m)}$ the coefficients of the m-th commutator defined recursively by

$$
(\mathcal{Z}_F^{(2)})_m \circ H^{(3)} \doteq [\,\mathcal{Z}_F^{(2)}, (\mathcal{Z}_F^{(2)})_{m-1} \circ H^{(3)}\,]
\tag{3.79}
$$

with $m \geq 1$, $(Z_F^{(2)})_o \circ H^{(3)} = H^{(3)}$, $b_4^{(m)} = V\,\delta_{m0}$, and arrange them in a vector array. Upon defining the transfer matrices $\mathbf{F}$, $\mathbf{B}$, and $\mathbf{Q}$ by

$$
\begin{aligned}
|\,b^{(m+1)} > &= \mathbf{F}\,|\,f^{(m)} >, \quad |\,f^{(m+1)} > = \mathbf{B}\,|\,b >^{(m)} \quad, \\
|\,f^{(m+2)} > &= \mathbf{Q}\,|\,f^{(m)} >, \quad \mathbf{Q} = \mathbf{BF} \quad,
\end{aligned}
\tag{3.80}
$$

we obtain, after some straightforward algebraic manipulations,

$$
\mathbf{Q} = \bar{\theta}\theta \begin{pmatrix} \sigma^2 & -\rho\sigma \\ -\rho\sigma & \rho^2 \end{pmatrix}.
\tag{3.81}
$$

Defining $z^2 = \bar{\theta}\theta(\rho^2 + \sigma^2)$, we have $\mathbf{Q}^k = z^{2(k-1)}\mathbf{Q}$, and this gives

$$
|\,f > = \sum_{k \geq 0} \frac{1}{k!}\,|\,f^{(k)} > = |\,f^{(0)} > + |\,f^{(1)} > + (\bar{\theta}\theta)\,\Phi\,|\,F >
\tag{3.82}
$$

where

$$\Phi = \Phi_1 \left(\frac{\cosh z - 1}{z^2} \right) + \Phi_2 \left(\frac{\sinh z - z}{z^3} \right) \qquad (3.83)$$

$$\Phi_1 = V(\sigma\gamma - \rho\delta), \quad \Phi_2 = \rho\sigma(\varepsilon'_2 - \varepsilon'_1)$$

and

$$\mid f^{(0)} >= V \begin{pmatrix} \gamma \\ \delta \end{pmatrix}, \quad \mid f^{(1)} >= \begin{pmatrix} \rho(\varepsilon'_1 + V) \\ \sigma(\varepsilon'_2 + V) \end{pmatrix}, \quad \mid F >= \begin{pmatrix} \sigma \\ -\rho \end{pmatrix}. \qquad (3.84)$$

In an analogous way, we obtain for the bosonic coefficients:

$$\mid b > = \sum_{k \geq 0} \frac{1}{k!} \mid b^{(k)} >= \mid b^{(0)} > + \mid b^{(1)} > + \frac{1}{2} \mid b^{(2)} > \qquad (3.85)$$

$$+ (\bar{\theta}\theta)^2 \left[\Phi_1 \left(\frac{\sinh z - z}{z^3} \right) + \Phi_2 \left(\frac{\cosh z - 1}{z^4} - \frac{1}{z^2} \right) \right] \mid B >$$

where

$$\mid b^{(0)} > = \begin{pmatrix} \varepsilon'_1 \\ \varepsilon'_2 \\ 0 \\ V \end{pmatrix}, \quad \mid b^{(1)} >= V(\bar{\theta}\theta) \begin{pmatrix} -2\sigma\,\delta \\ -2\rho\gamma \\ (\sigma\gamma + \rho\delta) \\ 0 \end{pmatrix},$$

$$\mid b^{(2)} > = \bar{\theta}\theta \begin{pmatrix} -2(\varepsilon'_2 + V)\sigma^2 \\ -2(\varepsilon'_1 + V)\rho^2 \\ \rho\sigma(\varepsilon'_1 + \varepsilon'_2 + 2V) \\ 0 \end{pmatrix}, \quad \mid B >= \begin{pmatrix} 2\sigma\rho \\ -2\sigma\rho \\ \sigma^2 - \rho^2 \\ 0 \end{pmatrix}. \qquad (3.86)$$

The diagonal hamiltonian is of course obtained by solving the system of two non-linear equations in ρ and σ defined by $\mid f >= 0$. The solutions $\tilde{\rho}$ and $\tilde{\sigma}$ have then to be successively inserted in the expression (3.85) in order to give the corresponding vector $\mid \tilde{b} >$.

Final step is to rotate $H^{(4)}$ into the Cartan sector of $\mathcal{B}$, i.e. to eliminate B_3. This is easily done selecting p_3 in $Z_B^{(3)}$ such that $\tan 2p_3 = 2\tilde{b}_3/(\tilde{b}_1 - \tilde{b}_2)$. We end up with a diagonal hamiltonian $\mathcal{H}$ given by

$$\mathcal{H} = h_1 N_1 + h_2 N_2 + V N_1 N_2 + C \qquad (3.87)$$

where

$$h_1 = \frac{1}{2}(\tilde{b}_1 + \tilde{b}_2 + \eta\sqrt{\Delta}) \quad, \quad h_2 = \frac{1}{2}(\tilde{b}_1 + \tilde{b}_2 - \eta\sqrt{\Delta}) \quad,$$

$$\eta = sgn(\tilde{b}_1 - \tilde{b}_2) \qquad (3.88)$$

$$\Delta = (\tilde{b}_1 - \tilde{b}_2)^2 + 4\tilde{b}_3^2 \quad.$$

According to the general discussion of the previous paragraph, we are now able to evaluate the partition function, and hence the expectation value of any operator $\in S$. In particular, we notice that the homogeneous case turns out to be simpler also for what concerns the self-consistency equations. Indeed, the two constraints on the θ_α's reduce to a single one, for the mean-field parameter $\theta\bar\theta$. The resulting equation, nevertheless, is highly non linear, and has to be solved simultaneously with the filling equation. In general, one ends up with a system of two equations which in principle has many different solutions. We treat then $\bar\theta\theta$ as a variational parameter, assuming that the physical solution is to be chosen as that minimizing the free-energy f, $f \doteq -\frac{1}{\beta}\ln Z$.

The numerical results for free-energy, mean-field parameter as well as some thermodynamical properties of the homogeneous solution of the model given by 3.5) are discussed in the next section.

3.5.1   Results and discussion

In figure 3.1, we report the order parameter $\bar\theta\theta$ as a function of the temperature T at half filling and for different values of V. The results refer to $q = 4$, (e.g. a square lattice in two dimensions), and to typical values of the physical parameters U and t. Noticeably enough, it appears that, beside to an intermediate-temperature phase, already discussed in [10], a non-vanishing V determines the appearence of a new low-temperature phase. In the low-temperature regime, there exist two different non-zero solutions to the self-consistency equation for $\bar\theta\theta$ for each T, corresponding to the two different ways the system has to realize a configuration with a given value of n_B. Indeed, as the hamiltonian (3.5) commutes separately with D_1 and D_2, the system itself is not capable of evolving dynamically from a configuration with a certain distribution of D_i's to another one, realizing the same m. Hence the different solutions at a given temperature may coexist, and the system may exhibit phase separation.

The extra low-temperature phase can be understood keeping in mind the relationship intercurring between the existence of non vanishing mean-field order parameters and the breaking of symmetries. As discussed in sections(1.4) and (2.3), the appearence of order parameters is natural whenever some of the symmetries of the original hamiltonian are broken by the linearized hamiltonian. In the present case, the linearized model does no longer commute with $\sum_i N_i$. Following the procedure illustrated in section(2.3), one should identify the correct order parameters with the expectation values of those operators $\in S$ which are not generated by commutation
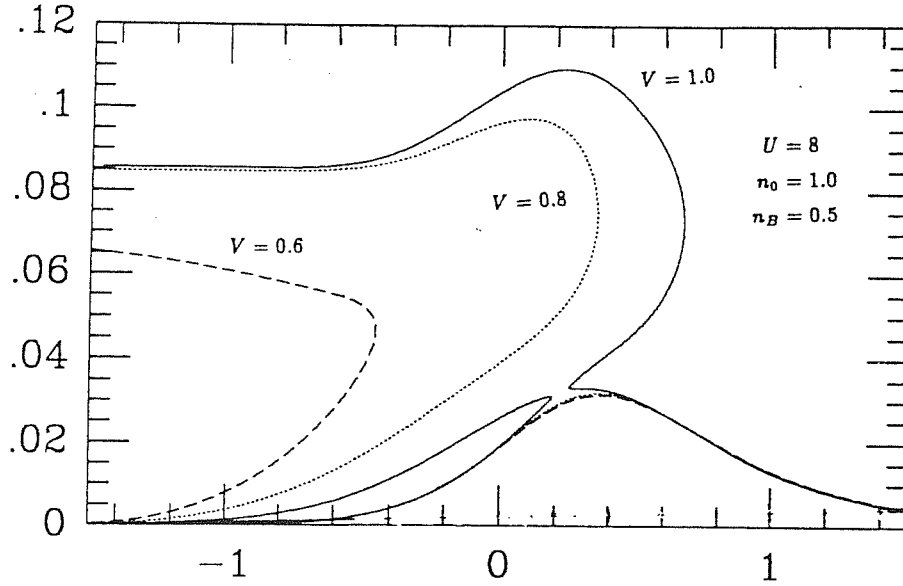
Figure 3.1: $\bar{\theta}\theta$ vs $\ln(k_B T)$ at half filling for fixed U and for various V

of H_d with S itself. One can check that, when $V = 0$, the dynamical algebra is smaller than S, and the above procedure leads to recognizing a single order parameter, $\mathcal{P}_1 \doteq < \bar{\theta}(A_1 + A_2) + (A_1^\dagger + A_2^\dagger)\theta >$, which describes the hopping between neighbouring dimers. On the contrary, when $V \neq 0$, the independent order parameters turn out to be two, $\mathcal{P}_1$ as well as $\mathcal{P}_2 \doteq < \bar{\theta}(N_2 A_1 + N_1 A_2) + (N_2 A_1^\dagger + N_1 A_2^\dagger)\theta >$, the latter referring to the hopping between neighbouring clusters when one of them is already occupied. In this case, $\bar{\theta}\theta$ keeps track of both of the corresponding phases.

Figure 3.1 shows that the low-temperature phase is much more sensitive to variations of V than the intermediate-temperature phase, for which in practice $\bar{\theta}\theta$ remains unchanged, at least in the range of V studied. According to the above discussion, the low-temperature phase appears to be related to $\mathcal{P}_2$. However, this is in agreement as well with the intuitive consideration that the greater is the Coulomb repulsion between neighbouring sites, the more an electron on a dimer is forced to hop out of the cluster if the other site of the dimer is occupied. Consequently, the intermediate temperature phase is described by $\mathcal{P}_1$.

In figure 3.2 we reported the behavior of $\bar{\theta}\theta$ in the low temperature phase for different values of the average number of fixed electrons, n_B, and the same total number of electrons ($n_0 = 1$). One can observe that, for n_B close to 0 or 1, the two branches of the curve tend to coincide, since there is only one possible distribution
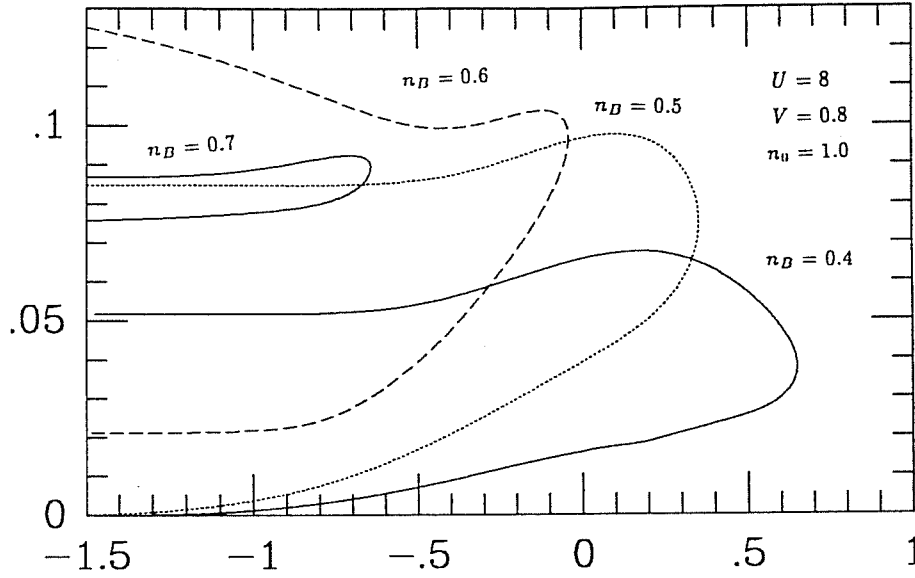
Figure 3.2: $\bar{\theta}\theta$ vs $\ln(k_B T)$ at half filling for fixed U and V and for various values of the average number of non-itinerant electrons n_B

of the D_i's which realizes the limiting values $n_B = 1$ or $n_B = 0$. Furthermore, one may identify the critical temperature T_c, as the temperature at which the two low-temperature branches collapse into a single point.

In figure 3.3, $\bar{\theta}\theta$ is reported versus temperature for various value of filling n_0, at a fixed value of V. Notice that both the low and the intermediate temperature phases seem to be very sensitive to variations of the filling, and it exists a critical value for n_0 above which the system always prefers the solution $\bar{\theta}\theta = 0$.

Finally, figure 3.4 shows the behavior at half filling of the local magnetic moment $< S^2 >$, which for the Hubbard model was already studied numerically in 1-d[69], and in 2-d[37]. The local magnetic moment is defined as

$$< S^2 >= \frac{3}{4} < \sigma_z^2 >\doteq \frac{3}{4} < (n_{i,\uparrow} - n_{i,\downarrow})^2 >= \frac{3}{4}(n_0 - 2 < N_i D_i >) \quad , \qquad (3.89)$$

where obviously at half-filling $n_0 = 1$. The two curves reported in figure refers to $V = 0$ and $V = 0.8$ respectively. Notice how the curves are continuous and smooth in correspondence of the transition between the two different non-zero regimes for $\bar{\theta}\theta$. This is not surprising because S^2 is a on-site operator, whereas $\bar{\theta}\theta$ is thought to describe non-local correlation. In fact, as seen before, $< S^2 >$ was not identified as an order parameter.

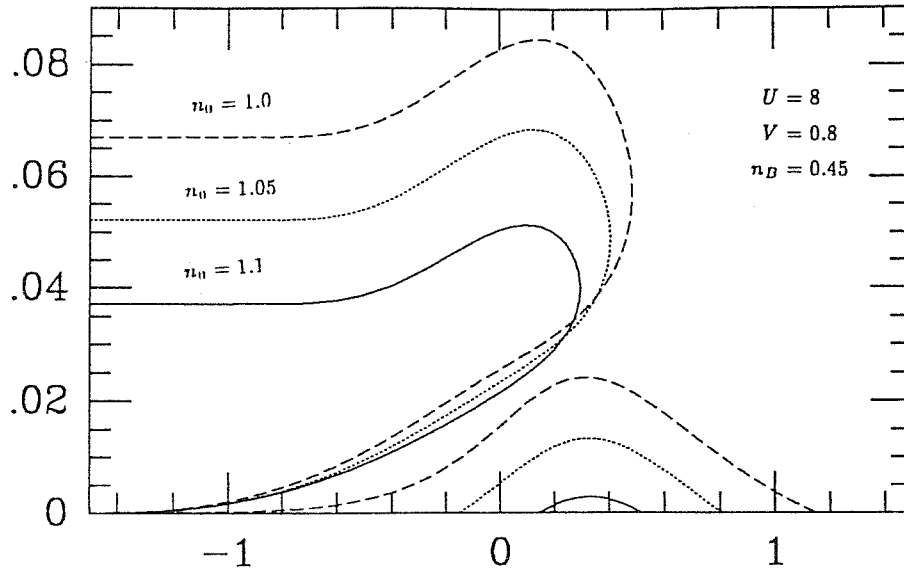Figure 3.3: $\bar{\theta}\theta$ vs $\ln(k_BT)$ at fixed U, V and n_B values, and for various values of the total filling n_0
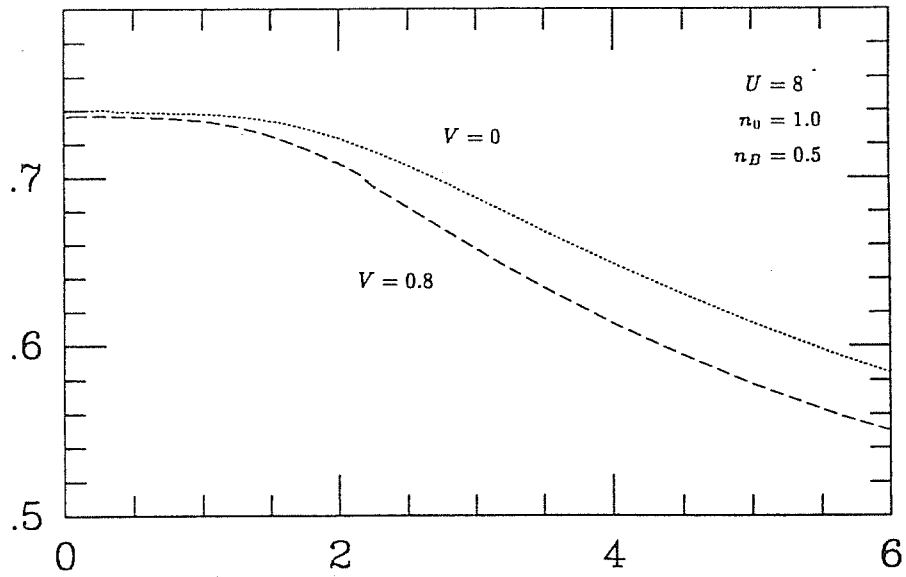

Figure 3.4: Local magnetic moment $< S^2 >$ vs k_BT at half-filling for fixed U and for different values of V

We conclude that the main feature that emerges, due to the presence of the intersite Coulomb repulsion, is the appearence of an extra (with respect to the $V = 0$ case) order parameter, which is proportional to the hopping expectation value in presence of other electrons. For low-temperatures, the latter describe a phase which is sensitively dependent on the value of V, as well as on the total filling.

The homogeneous solution presented here is not the more general solution to the problem described by the model hamiltonian. In particular, we expect that a solution with a different symmetry, *i.e.* $\theta_1 = \bar{\theta}_2 \equiv \theta$, which gives non-vanishing pairing, would minimize the free-energy for certain values of the parameters. However, the study of such a solution present non-trivial numerical problems and no results have been obtained up to now.

Chapter 4

The Clifford Mean-Field Approximation

4.1 Introduction

In the present chapter, another view of the fermionic linearization scheme is illustrated. It consists in requiring that the mean-field amplitudes are treated as fermionic operators instead of elements of a Grassmann-like algebra. More precisely, calling ϑ_i these variables, they satisfy a Clifford-like algebra:

$$\{ \vartheta_i, \bar{\vartheta}_j \} = c_i\, \delta_{ij} \quad , \quad c_i \in \mathbb{R} \tag{4.1}$$

where c_i are undeterminates to be defined for each specific problem.

First of all, we notice that (4.1) implies that the dynamical algebra of the linearized model is no longer graded, but simply a Lie algebra. Secondly the values of the c_i's have to be determined self-consistently or in a variational way. As we will see later, the definitions for the approximate expression for multilinears and consequently for the self-consistency equations are not unique, and this can give rise to different linearized models.

In section (4.2), we will analize the algebraic structure of the Hubbard model with some numerical results for the Falicov-Kimball as special case (section 4.3). Then in section (4.4), we give the dynamical structure of the extended Falicov-Kimball.

4.2   The Hubbard model

In the previous sections, we have used the fermionic linearization scheme acting only on the hopping term of the Hubbard hamiltonian

$$H_H = -\mu \sum_i (n_{i,\uparrow} + n_{i,\downarrow}) - t \sum_{<i,j>} \sum_\sigma (a^\dagger_{i,\sigma} a_{j,\sigma} + a^\dagger_{j,\sigma} a_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \qquad (4.2)$$

through the relation $(A_i \equiv a_{i,\sigma},\ \sigma = \uparrow, \downarrow)$

$$A^\dagger_i A_j \simeq \bar\eta A_j + A^\dagger_i \eta - \bar\eta \eta \qquad (4.3)$$

where η and $\bar\eta$ were Grassmann-like variables. In this chapter we will use a somewhat different approximation. Let us write

$$\sum_{<i,j>} A^\dagger_i A_j = \frac{q}{2} \sum_i (\vartheta^\dagger_i A_i + A^\dagger_i \vartheta_i) \quad , \qquad (4.4)$$

with $\vartheta_i = q^{-1} \sum_{j\ n.n.i} A_j$ and q is the number of nearest neighbours of a site in the lattice. In this case, we will improve the fermionic linearization scheme by directly replacing the operators ϑ_i by variable Θ_i still anticommuting with the fermion operators which are locally Clifford variables:

$$\Theta^2_i = \bar\Theta^2_i = 0 \quad , \quad \{\Theta_i, \bar\Theta_j\} = c\ \delta_{ij} \quad . \qquad (4.5)$$

Once the above approximation is inserted, one obtains a reduced Hubbard hamiltonian $\mathcal{H}$ which is a sum over lattice sites of single-particle hamiltonians $H^{(i)}$ commuting with each other. Defining the new variables

$$A_1 := a_{i\uparrow}, \quad A_2 := a_{i\downarrow}, \quad A_3 = \Theta_i / \sqrt{c} \qquad (4.6)$$

so that $\{A_3, A^\dagger_3\} = 1$, we obtain

$$H^{(i)} = -\mu(N_1 + N_2) + U N_1 N_2 - tq\sqrt{c}\ [(A^\dagger_1 + A^\dagger_2)A_3 + \text{h.c}] \qquad (4.7)$$

where the index i has been omitted.

The closure under Lie bracket of the operators appearing in (4.7) leads to the dynamical algebra $\mathcal{A}_H$,

$$\mathcal{A}_H = \bigoplus_{k=1}^{4} u_k(1) \oplus su(3) \oplus su(3). \qquad (4.8)$$

The four central elements C_l generating the $u(1)$'s are given by:

$$C_0 = \mathbb{I} \quad , \quad C_1 = N_1 + N_2 + N_3 \quad ,$$
$$C_2 = N_1 N_2 + N_1 N_3 + N_2 N_3 \quad , \quad C_3 = N_1 N_2 N_3 \quad . \tag{4.9}$$

The Cartan-Weyl basis $\{H_i, E_\alpha\}$ of the first $su(3)$ subalgebra of $\mathcal{A}_H$ is given by:

$$E_1 = N_3 A_1^\dagger A_2 \quad , \quad E_2 = N_1 A_2^\dagger A_3 \quad , \quad E_3 = N_2 A_1^\dagger A_3$$
$$E_{-1} = N_3 A_2^\dagger A_1 \quad , \quad E_{-2} = N_1 A_3^\dagger A_2 \quad , \quad E_{-3} = N_2 A_3^\dagger A_1 \tag{4.10}$$
$$H_1 = \frac{1}{\sqrt{2}} N_3 (N_1 - N_2) \quad , H_2 = \frac{1}{\sqrt{6}} (N_1 (N_2 - N_3) + N_2 (N_1 - N_3))$$

and

$$\alpha_1 = \frac{1}{\sqrt{2}}(2,0) \quad , \quad \alpha_2 = \frac{1}{\sqrt{2}}(-1, \sqrt{3}) \quad , \quad \alpha_3 = \frac{1}{\sqrt{2}}(1, \sqrt{3}) \quad . \tag{4.11}$$

The other $su(3)$ Lie algebra is defined by the "orthogonal" set of operators $\{\tilde{H}_i, \tilde{E}_\alpha\}$ defined by the substitution $N_i \rightarrow (1 - N_i)$ for the N_i multiplying the fermionic bilinears in the set $\{E_\alpha\}$ and the differences $N_i - N_j$ in the Cartan subset $\{H_1, H_2\}$.

In terms of the operators define above, and making the further assumption that $\mu_1 = \mu_2 = \mu$ (i.e. $\varepsilon_{i\uparrow} = \varepsilon_{i\downarrow}$ and $n_{i\uparrow} + n_{i\downarrow}$ is kept fixed), $H^{(i)}$ can be rewritten as

$$H^{(i)} = \mathcal{H}_{u(1)} \oplus \mathcal{H}_{su(3)}^{(1)} \oplus \mathcal{H}_{su(3)}^{(2)} \quad . \tag{4.12}$$

with

$$\mathcal{H}_{u(1)} = -\frac{1}{3}(2\mu + tc)C_1 + \frac{1}{3}UC_2 \quad ,$$
$$\mathcal{H}_{su(3)}^{(1)} = \frac{2}{\sqrt{6}}(-\mu + U)H_2 - qt\sqrt{c}(E_2 + E_{-2} + E_3 + E_{-3}) , \tag{4.13}$$
$$\mathcal{H}_{su(3)}^{(2)} = -\frac{2}{\sqrt{6}}\mu\tilde{H}_2 - qt\sqrt{c}(\tilde{E}_2 + \tilde{E}_{-2} + \tilde{E}_3 + \tilde{E}_{-3}) \quad .$$

Now we proceed to the diagonalization of $\mathcal{H}$. Let us write H as a general hermitian element in the first $su(3)$ CW-basis:

$$H = \varepsilon_1 H_1 + \varepsilon_2 H_2 + \tau(E_2 + E_{-2} + E_3 + E_{-3}). \tag{4.14}$$

Due to the fact that in our particular case, see equation (4.13), $\varepsilon_1 = 0$, with $Z_1 = (-\frac{\pi}{4})(E_1 - E_{-1})$, we reduce H to

$$H' = \exp(\mathrm{ad}Z_1)(H) = \varepsilon_2 H_2 + \sqrt{2}\tau(E_2 + E_{-2}) \tag{4.15}$$

and therefore $H' \in u(2) = \{H_1, H_2, E_2, E_{-2}\}$. Now, we can use the procedure shown in section (1.3) to diagonalize H'. We define the ket $\mid \Phi^{(k)} >= \mid \beta_1^{(k)}, \beta_2^{(k)}, \mu^{(k)} >$ with $\beta_1^{(0)} = 0$, $\beta_2^{(0)} = \varepsilon_2$, $\mu^{(0)} = \sqrt{2}\tau$ and $\mid H' >= \mid H_1, H_2, E_+ >$, $E_+ \equiv E_2 + E_{-2}$ such that $H' =< \Phi^{(0)} \mid H' >$. With $Z_2 = \phi(E_2 - E_{-2})$, we define the recursive relation $H'^{(k)} = [Z_2, H'^{(k-1)}] =< \Phi^{(k)} \mid H' >$. This brings to the definition of the 3×3 matrix A

$$A = \begin{pmatrix} 0 & 0 & -2a \\ 0 & 0 & 2b \\ a & -b & 0 \end{pmatrix} \quad , \quad a = \frac{\phi}{\sqrt{2}} \quad , \quad b = \sqrt{\frac{3}{2}}\phi \qquad (4.16)$$

for which $\mid \Phi^{(k+1)} >= A \mid \Phi^{(k)} >$. The rotated hamiltonian H'' can then be written as

$$H'' = \exp(\mathrm{ad}Z_2)(H') =< \Phi^{(0)} \mid e^A \mid H' > \qquad (4.17)$$

where

$$e^A = \frac{1}{4} \begin{pmatrix} \cos 2\phi + 3 & -\sqrt{3}(\cos 2\phi - 1) & -2\sqrt{2}\sin 2\phi \\ -\sqrt{3}(\cos 2\phi - 1) & 3\cos 2\phi + 1 & 2\sqrt{6}\sin 2\phi \\ \sqrt{2}\sin 2\phi & \sqrt{6}\sin 2\phi & \cos 2\phi \end{pmatrix} \quad . \qquad (4.18)$$

Equating to zero the resulting coefficient of the non-diagonal element E_+ gives for the rotation angle ϕ the effective value

$$\tilde{\phi} = \frac{1}{2}\arctan\frac{4\tau}{\sqrt{3}\varepsilon} \qquad (4.19)$$

and we obtain, inserting this value in (4.17), the diagonalized hamiltonian

$$\begin{aligned} \tilde{H}'' &= \exp(\mathrm{ad}Z_2)\exp(\mathrm{ad}Z_1)(H) \\ &= \frac{1}{4}(\sqrt{3}\varepsilon_2 - \sqrt{\Delta})\,H_1 + \frac{1}{4}(\varepsilon_2 - \sqrt{3\Delta})\,H_2 \quad , \end{aligned} \qquad (4.20)$$

with $\Delta := 3\varepsilon_2^2 + 16\tau^2$. The partition function can be immediately obtained from (4.20) as

$$\mathcal{Z} = \sum_{N_1,N_2,N_3=0,1} \exp(-\beta\,\tilde{H}'') \quad . \qquad (4.21)$$

Predictions for physical quantities can then be obtained from $\mathcal{Z}$ once the average number of electrons n_0 are fixed through the chemical potential according to

$$n_0 =< N_1 + N_2 >= \frac{1}{\beta\mathcal{Z}}\frac{\partial \mathcal{Z}}{\partial\mu} \qquad (4.22)$$

where as usual $< \hat{O} >$ stays for the thermodynamical average in the Gibbs ensemble of the operator $\hat{O}$.

Morever, in order to have quantitative predictions, a numerical value for c has still to be self-consistently determined. One possibility is to implement relation (4.4) giving rise to

$$< A_3^\dagger A_i + A_i^\dagger A_3 > = 2\sqrt{c} < A_3^\dagger A_3 > \qquad (4.23)$$

where translational invariance of the lattice has been assumed.

4.3 The Falicov-Kimball model

In this section we give some explicit results about a simplified version of the Hubbard model already introduced in chapter 3, namely the Falicov-Kimball model in which only one species of electrons itinerates, the electrons with opposite spin being fixed at their sites [52]. The hamiltonian (4.7) simplifies to

$$H_{FK}^{(i)} = -\mu_A N_i - \mu_B D_i + U\, D_i N_i - tq\sqrt{c}\ (\bar{\eta} A_i + A_i^\dagger \eta) \quad . \qquad (4.24)$$

In this notation, $A_i^\dagger$ and A_i are creation and annihilation operators of the itinerant electrons ($N_i = A_i^\dagger A_i$), while D_i is the number operator of the non-itinerant electrons. Respect to (4.7), omitting the site index i, this implies the change of notation $N_1 \rightarrow N$, $N_2 \rightarrow D$, $A_3 \rightarrow \eta$. As the operators $\sum_i N_i$ and $\sum_i D_i$ both commute with the hamiltonian, we introduced the chemical potentials μ_A and μ_B in order to fix the average number of electrons of the two species. As in section (3.2), the D_i's are to be considered as classical Ising-like variables, whose two possible eigenvalues 0 and 1 label the two orthogonal projections of $H_{FK}^{(i)} = H^{0)} \oplus H^{(1)}$. It is easy to check that the dynamical algebra $\mathcal{A}_{FK}$ of (4.24) coincides with the Lie algebra $u(2)$ generated by

$$\mathcal{A}_{FK} = \{N_i \pm \bar{\eta}\eta, \bar{\eta}A \pm A\eta\}. \qquad (4.25)$$

A rotation similar to (4.17) leads to the diagonal form

$$\tilde{H}_{FK} = \frac{1}{2}\{\varepsilon_i(\bar{\eta}\eta + N_i) \pm \sqrt{\varepsilon_i^2 + 4\tau^2}(\bar{\eta}\eta - N_i)\} - \mu_B D_i \qquad (4.26)$$

with $\varepsilon_i = U D_i - \mu_B$. The analogon of (4.21),(4.22) and (4.23) are now

$$\mathcal{Z} = \sum_{N_i, D_i, \bar{\eta}\eta = 0, 1} \exp(-\beta\, \tilde{H}_{FK}) \quad , \qquad (4.27)$$

$$n_A = < N_i > = \frac{1}{\beta\mathcal{Z}}\frac{\partial\mathcal{Z}}{\partial\mu_A} \quad , \qquad (4.28)$$

$$n_B = <D_i> = \frac{1}{\beta \mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \mu_B} \quad , \tag{4.29}$$

$$<\bar{\eta} A_i + A_i^\dagger \eta> = 2\sqrt{c} <\bar{\eta}\eta> \quad . \tag{4.30}$$

4.3.1 Results and discussion

In figure 1. we report the mean-field parameter c vs. temperature $\frac{kT}{qt}$, at half-filling and for the symmetric case $n = d = \frac{1}{2}$. In this case it is easy to check that the solution to (4.28)–(4.29) is $\mu_n = \mu_d = \frac{U}{2}$. c is plotted for different U values, and exhibits a typical order-parameter like behavior. For $U = 0$ (non-interacting case) it rises from zero, in the high-temperature regime, to one, at $T = 0$. For generic $U \leq 4qt$, it is possible to show rigorously that, in the limit $T \to 0$, c reaches a value c_0 given by

$$c_0^2 = 1 - \frac{1}{16}\bar{U}^2 \quad , \tag{4.31}$$

where $\bar{U} \doteq \frac{U}{qt}$. This suggests that the value $c = 1$ used in [63] is correct at half filling, only in a low-temperature non-interacting regime or for $D = \infty$. On the contrary, for $U > 4qt$, the only solution to (4.30) is $c = 0$.

The expression (4.31) for c_0 clarifies the physical meaning of the parameter c. Indeed, recalling that on a hypercubic lattice q is twice the dimension of the lattice, equation (4.31) reproduces exactly the Gutzwiller result [36] for the discontinuity in the single particle occupation number at the Fermi surface, obtained for the conventional Hubbard model when $T = 0$. This is not surprising as, on the one hand, the Gutzwiller result for the Hubbard model was obtained in fact by neglecting the kinetic energy of one species of electron, thus in an approximation very similar to that at the basis of the Falicov-Kimball model. On the other hand, according to eqs. (4.4), (4.5), and (4.30), at half filling c coincides with the expectation value of the hopping term, and hence is related to the discontinuity in its Fourier transform.

Notice that when $U = 0$ then $c_0 = 1$, and the ground state has all the electrons below the Fermi level. For any $c \neq 0$, the ground state has some electrons above the Fermi level, but the gap is still there, and, according to eq. (4.5), the generic lattice site on which one has confined the linearized hamiltonian is still interchanging fermions with the rest of the lattice. When $c_0 = 0$ on the other hand, the gap in the density of states disappears, and at half-filling we have exactly one electron per site. In this case, the remaining of the lattice behaves as a system of scorrelated 'average' fermions (*i.e.* as if they were frozen at their own sites) and we are in presence of an
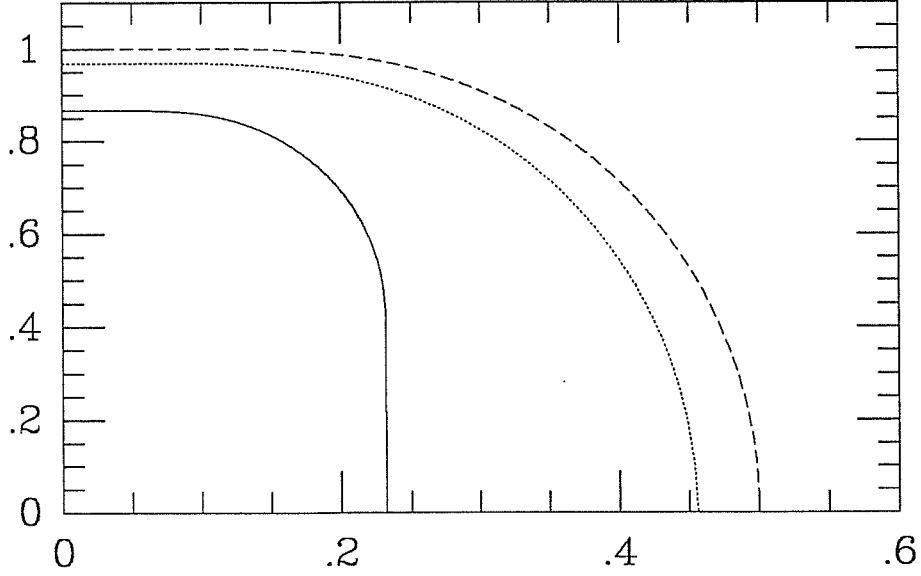
Figure 4.1: c vs $(k_B T/qt)$ at different $\tilde{U}$ values: $\tilde{U} = 0$ (dashed line), $\tilde{U} = 1$ (dotted line), $\tilde{U} = 2$ (continuous line)

insulating phase.

The above analysis suggests that c could be able to describe the transition from a conducting to an insulating state. Indeed, again in agreement with the Gutzwiller result, at $T = 0$ one finds that the double occupancy expectation value, $\mathcal{P} \doteq <N_i D_i >$, vanishes precisely at $\tilde{U} = 4$. Explicitly, analytic calculation shows that

$$\mathcal{P} = \begin{cases} \dfrac{1}{4}\left(1 - \dfrac{\tilde{U}}{4}\right) & \text{for } \tilde{U} \leq 4 \\ 0 & \text{otherwise} \end{cases} \tag{4.32}$$

It is worth noticing that the result (4.32) coincides with the exact result both in the limit $\tilde{U} = 0$ and in the limit $\tilde{U} >> 1$. A deeper analysis of figure 4.1. shows that

the transition from non-zero to vanishing c is of different order depending on the value of $\tilde{U}$. Indeed, by requiring that (4.30) vanishes also around $|c| = 0$, one can
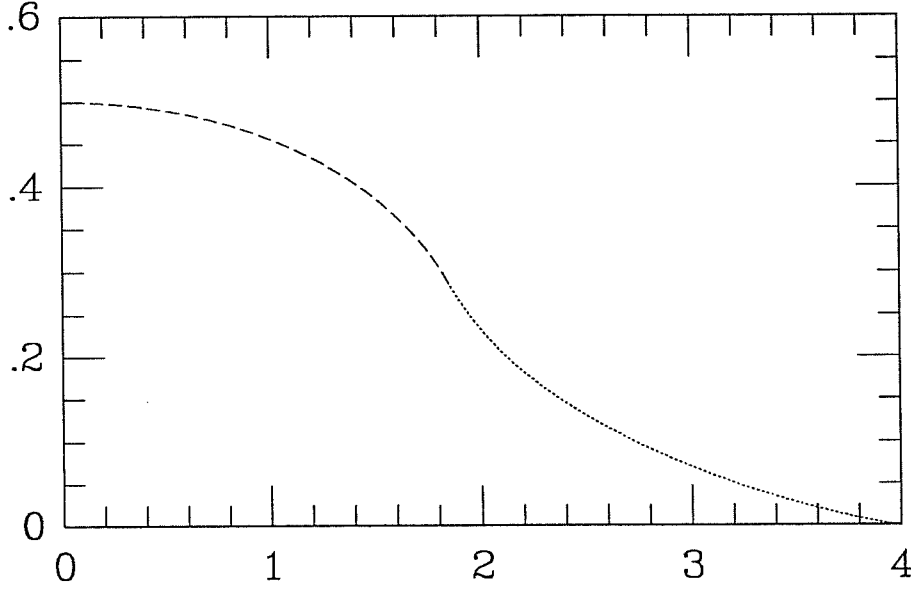
Figure 4.2: $(k_B T_c/qt)$ vs $\tilde{U}$: dashed line represents second order transition, dotted line first order transition.
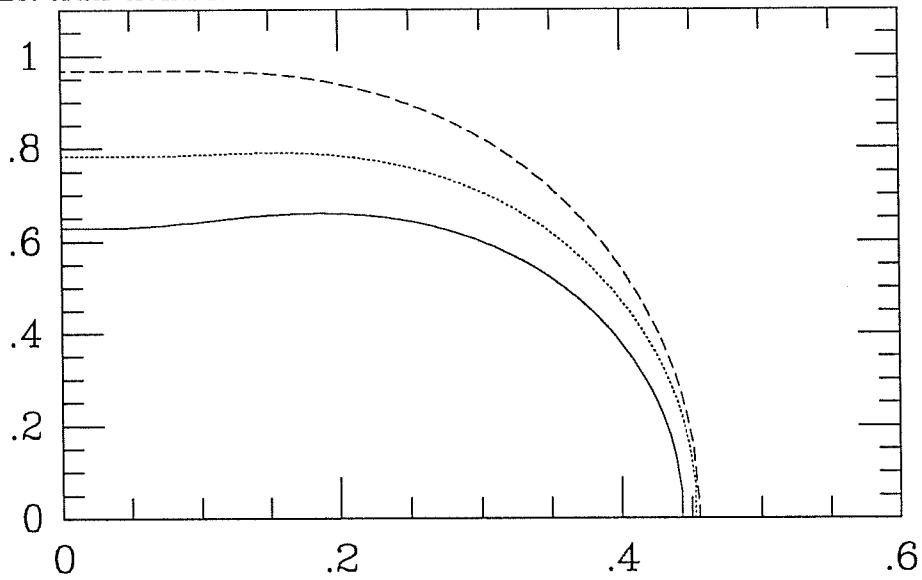

Figure 4.3: c vs $(k_B T/qt)$ at $\tilde{U} = 1$ and different fillings, in the neutral case $(n = d)$: $n + d = 1$ (dashed line), $n + d = 0.8$ (dotted line), $n + d = 0.6$ (continuous line)

verify that there exists a tri-critical point at $\tilde{U} = U_t$, where U_t is solution of

$$\tanh \frac{U_t}{2\left(1 - \frac{U_t^2}{8}\right)} = \frac{U_t}{2} \quad . \tag{4.33}$$

One finds a numerical value $U_t \simeq 1.845$. For $\tilde{U}$ smaller than U_t the transition is second order, and the critical temperature is found analytically as the solution T_c of the following equation (obtained by requiring that (4.30), upon factorizing the $c = 0$ solution, still vanishes for $c = 0$):

$$\tanh \frac{\tilde{U}}{4\Theta_c} = \frac{\tilde{U}}{2} \quad , \tag{4.34}$$

with $\Theta_c \doteq \frac{k_B T_c}{qt}$, and k_B the Boltzmann constant. On the other hand, when $\tilde{U}$ is larger than U_t, the transition is first order, and the critical temperature can be evaluated numerically. Figure 4.2 shows the behavior of T_c vs. $\tilde{U}$ in the two regions. The value $\tilde{U} = 4$ correspond to the vanishing of both the critical temperature and c_0.

Figure 4.2 can be compared with the rough estimate of the critical temperature of the long-range order phase whose existence is proved for the Falicov-Kimball model in [43]. If one assumes that the phase with $c \neq 0$ could possibly be the long range order phase, the qualitative behavior of T_c is in agreement with that given in [43] for large U, whereas it is in contrast with the latter for vanishing U. One should notice however that this approximation is expected to be more realistic for finite U.

Finally, in figure 4.3 we give the behavior of c vs. T for various fillings, still for a paramagnetic state (n=d). The figure shows that the transition is present at different fillings, again in agreement with the features of the long-range ordered phase described in [43]

The above results suggest that the approximation could be a natural extension of the Gutzwiller approach to the case $T \neq 0$. They also provide a physical interpretation to the method, which consists in replacing the hopping term by a term which locally still allows to create and annihilate electrons, but with an amplitude proportional to the discontinuity in the single particle average number at the Fermi surface.

Moreover, as opposite to the case in which the coefficients of the linearized operators were Grassmann variables, the present approximation produces non-trivial results even in the case $U = 0$.

4.4 Extended Falicov-Kimball model

In this section we study the structure of dynamical symmetry which the use of Clifford-like mean-fields defined in the previous sections leads to, in the case of the extended Falicov model introduced in chapter 4 [22]. We rewrite the linearized hamiltonian $\mathcal{H}_D$ in the form

$$
\begin{aligned}
\mathcal{H}_D \;=\; & \sum_{\alpha=1}^{2} \varepsilon_\alpha N_\alpha + V N_1 N_2 + t \left(A_1^\dagger A_2 + A_2^\dagger A_1 \right) + \tilde{C} \\
& + \sum_{\alpha=1}^{2} \left(A_\alpha^\dagger \Theta_\alpha + \bar{\Theta}_\alpha A_\alpha \right) \quad,
\end{aligned}
\tag{4.35}
$$

with

$$
\begin{aligned}
\Theta_\alpha \;=\;& t \sum_{\substack{\beta n.n.\alpha \\ \beta \neq \alpha}} A_\beta \quad, \\
\varepsilon_\alpha \;=\;& -\mu_A + V n_0 (q-1) + U D_\alpha + V D_{\bar\alpha} \doteq \mathcal{E} + \mathcal{W}_\alpha \quad, \\
\tilde{C} \;=\;& (\mathcal{E} + \mu_A - \mu_B)(D_1 + D_2) + V D_1 D_2 - V(q-1)n_0^2 \quad,
\end{aligned}
\tag{4.36}
$$

q being the number of n.n. sites per site in Λ and $\bar\alpha \equiv \alpha + 1 \,(\mathrm{mod}\,2)$.

Let us rewrite explicitly the properties of the variables $\{\Theta_\alpha\,,\,\bar\Theta_\alpha \mid \alpha = 1,2\}$:

- the generators $\{\Theta_\alpha, \bar\Theta_\alpha | \alpha \in \mathcal{D}\}$ anticommute with all fermion operators:

- $\{A_\beta, \Theta_\alpha\} = 0 = \{A_\beta^\dagger, \Theta_\alpha\} = 0 = \{A_\beta, \bar\Theta_\alpha\} = 0 = \{A_\beta^\dagger, \bar\Theta_\alpha\}, \forall \alpha, \beta \in \mathcal{D}$;

- the generators $\{\Theta_\alpha, \bar\Theta_\alpha | \alpha \in \mathcal{D}\}$ anticommute between each other for $\alpha \neq \beta$:
  $\{\Theta_\alpha, \Theta_\beta\} = 0 = \{\bar\Theta_\alpha, \bar\Theta_\beta\} = 0 = \{\Theta_\alpha, \bar\Theta_\beta\} = 0 = \{\bar\Theta_\alpha, \Theta_\beta\}$;

- locally the generators $\{\Theta_\alpha | \alpha \in \mathcal{D}\}$ are nilpotent Clifford variables:

- $\Theta_\alpha^2 = 0 = \bar\Theta_\alpha^2$, $\{\Theta_\alpha, \bar\Theta_\alpha\} = c_\alpha^2$, where the $\{c_\alpha\}$'s are c-numbers;

- $\bar\Theta_\alpha$ is the conjugate of Θ_α, $\forall \alpha \in \mathcal{D}$.

In other words, we introduce a mean field which <u>is</u> itself a fermionic <u>*operator*</u>.

Upon noticing how $\{\Theta_\alpha, \bar\Theta_\alpha | \alpha \in \mathcal{D}\}$ enter into play in $\mathcal{H}_D$, we introduce, besides the fermionic operators $A_\alpha, A_\alpha^\dagger$, $\alpha = 1, 2$ the auxiliary fermionic variables $A_{\lambda+2} \equiv$

$\frac{1}{c_\lambda} \Theta_\lambda$, $A_{\lambda+2}^\dagger \equiv \frac{1}{c_\lambda} \bar{\Theta}_\lambda$; $\lambda = 1, 2$. The linearized hamiltonian $\mathcal{H}_D$ will therefore be written in the form

$$\mathcal{H}_D = \sum_{\alpha=1}^{2} \varepsilon_\alpha N_\alpha + V N_1 N_2 + \frac{1}{2} \sum_{\nu=1}^{4} \sum_{\substack{\gamma=1 \\ \gamma \neq \nu}}^{4} \tau_{\nu,\gamma} A_\nu^\dagger A_\gamma \quad , \qquad (4.37)$$

where the antisymmetric matrix $\mathbf{T}$ of elements $\mathbf{T}_{\nu,\gamma} \equiv \tau_{\nu,\gamma}$ is given by

$$\mathbf{T} = \sigma_x \otimes [(c_1 + c_2)\mathbb{I}_2 + (c_1 - c_2)\sigma_z] + t (\mathbb{I}_2 + \sigma_z) \otimes \sigma_x \quad , \qquad (4.38)$$

σ_κ, $\kappa = x, y, z$ denoting the usual Pauli matrices. It is worth pointing out that ε_1 is in general ($V \neq U$) different from ε_2.

The form (4.37) of hamiltonian (4.35) is particularly interesting, in that it exhibits quite manifestly the whole set of dynamical symmetries characteristic of the system in its linearized form. In order to show this, we observe first that, in the absence of the V term, we should recover (with $n = 4$) the well known $su(n)$ symmetry characteristic of a system with n fermions, generated by all number conserving bilinear forms of creation and annihilation operators [14]. The n.n. Coulomb coupling term, $N_1 N_2$, can be expected to lead us to an extended dynamical algebra $\mathcal{A}_n$, generated by all number preserving multilinear forms of type $\{A_{\alpha_1}^\dagger \cdots A_{\alpha_n}^\dagger A_{\beta_1} \cdots A_{\beta_n}\}$, $n = 1, \ldots, 4$. One can show (by induction, after working out explicitly the cases $n = 2$ and $n = 3$) that in general such an algebra is

$$\mathcal{A}_n = \bigoplus_{\kappa=0}^{n} u_\kappa(1) \oplus \bigoplus_{\kappa=1}^{n-1} su\left(\binom{n}{\kappa}\right) \quad . \qquad (4.39)$$

In present application ($n = 4$) the dynamical algebra is therefore $\mathcal{A}_D \equiv \mathcal{A}_4 \equiv 5u(1) \oplus 2 \cdot su(4) \oplus su(6)$. $\mathcal{A}_D$ has 70 generators, 16 of which are Cartan, and 5 are central. These generators can naturally be straightforwardly obtained by commuting in all possible ways the operators entering $\mathcal{H}_D$.

Upon introducing the auxiliary variables $E_\beta^\alpha \doteq A_\alpha^\dagger A_\beta$ (notice that $E_\alpha^\beta = E_\beta^{\alpha \dagger}$, $E_\alpha^\alpha \equiv N_\alpha$), the generators of $\mathcal{A}_D$ turn out to be given by the following tensor operators:

$$F^{(l)\,\{\alpha_i\}}_{\quad \{\beta_i\}} := \prod_{i=1}^{l} E_{\beta_i}^{\alpha_i} \quad , \quad l = 1, 2, 3, 4 \quad , \qquad (4.40)$$

where the indices α_i, β_i all different from one another range from 1 to 4. The five central elements $\mathcal{C}_l$, generating the 5 $u(1)$'s, are given by:

$$\mathcal{C}_0 = 1 \quad , \quad \mathcal{C}_\ell = \sum_{\alpha_1 < \cdots < \alpha_l} \left(\prod_{i=1}^{\ell} N_{\alpha_i} \right) \quad , \quad \ell = 1, \ldots, 4 \quad . \qquad (4.41)$$

In order to recognize the direct product structure of the algebra, let us define the following set of tensor operators which are subsets of the $F^{(l)}$'s in (4.40):

$$J^\alpha_\beta \equiv N_\gamma N_\delta E^\alpha_\beta \quad ; \quad \hat{J}^\alpha_\beta \equiv (1 - N_\gamma)(1 - N_\delta)E^\alpha_\beta \quad ;$$

$$^\alpha_\beta P^\gamma_\delta \equiv E^\alpha_\beta E^\gamma_\delta \quad ; \quad ^\gamma_\delta M^\alpha_\beta \equiv N_\gamma(1 - N_\delta)E^\alpha_\beta \quad ; \tag{4.42}$$

where $\alpha \neq \beta$ and $\gamma \neq \delta$. In the first two relations of (4.42), we introduced the convention that whenever in the definition of some operator appear two extra indices besides those labelling the operator itself, one should think of them as assuming the complementary values in the set $\{1, 2, 3, 4\}$.

We may immediately obtain for J^α_β the commutation relations of $su(4)$:

$$[J^\alpha_\beta, J^\gamma_\delta] = \delta_{\beta\gamma} J^\alpha_\delta - \delta_{\alpha\delta} J^\gamma_\beta \quad ,$$

$$[J^\alpha_\beta, J^\beta_\alpha] = N_\gamma N_\delta(N_\alpha - N_\beta) \quad . \tag{4.43}$$

The first relation above holds whenever it is not simultaneously $\alpha = \delta$ and $\beta = \gamma$, in which case one should use the second.

Quite similar relations hold for and $\hat{J}^\alpha_\beta$ (upon replacing N_j with $(N_j - 1)$ in the second commutator of (4.43), generating the second $su(4)$, manifestly orthogonal – due to the presence of the projection operators – to the previous one.

Analogously, the algebra generated by the set $\{^\gamma_\delta M^\alpha_\beta, ^\gamma_\delta P^\alpha_\beta\}$ is:

$$[^\gamma_\delta M^\alpha_\beta, ^\rho_\sigma M^\mu_\nu] = \delta_{\beta\mu}(\delta_{\alpha\rho}\delta_{\gamma\nu} {}^\beta_\delta M^\alpha_\gamma + \delta_{\alpha\sigma}\delta_{\gamma\rho} {}^\gamma_\beta M^\alpha_\delta$$
$$- \delta_{\alpha\nu}(\delta_{\beta\rho}\delta_{\gamma\mu} {}^\alpha_\delta M^\gamma_\beta + \delta_{\beta\sigma}\delta_{\gamma\rho} {}^\gamma_\alpha M^\delta_\beta)$$
$$+ \delta_{\alpha\sigma}\delta_{\beta\rho}\delta_{\gamma\mu} {}^\alpha_\beta P^\gamma_\delta - \delta_{\alpha\rho}\delta_{\beta\sigma}\delta_{\gamma\nu} {}^\alpha_\beta P^\delta_\gamma \quad , \tag{4.44}$$

$$[^\gamma_\delta P^\alpha_\beta, ^\rho_\sigma P^\mu_\nu] = (\delta_{\beta\mu}\delta_{\delta\rho} - \delta_{\beta\rho}\delta_{\delta\mu})(\delta_{\alpha\nu} - \delta_{\alpha\sigma})$$
$$(N_\alpha N_\gamma(1 - N_\beta)(1 - N_\delta) - N_\beta N_\delta(1 - N_\alpha)(1 - N_\gamma)) \tag{4.45}$$

$$[^\gamma_\delta P^\alpha_\beta, ^\rho_\sigma M^\mu_\nu] = (\delta_{\alpha\nu}\delta_{\gamma\sigma}(\delta_{\beta\mu} - \delta_{\beta\rho}) + \delta_{\alpha\sigma}\delta_{\gamma\nu}(\delta_{\beta\mu} + \delta_{\beta\rho})) {}^\nu_\mu M^\sigma_\rho$$
$$+ (\delta_{\alpha\nu}\delta_{\gamma\rho}(\delta_{\beta\sigma} - \delta_{\beta\mu}) - \delta_{\alpha\rho}\delta_{\gamma\nu}(\delta_{\beta\mu} + \delta_{\beta\sigma})) {}^\mu_\nu M^\rho_\sigma \quad . \tag{4.46}$$

which can be easily recognized to be isomorphic with that of $su(6)$ (see appendix D).

The operators $E_1 \doteq J^1_2$, $E_2 \doteq J^3_4$, $E_3 \doteq J^2_3$, $E_4 \doteq J^1_3$, $E_5 \doteq J^2_4$, $E_6 \doteq J^1_4$ and the analogous $\hat{E}_\kappa$, defined with the $\hat{J}$'s, together with

$$H_1 \doteq \frac{1}{2}(N_1 N_4(N_2 - N_3) + N_2 N_3(N_1 - N_4)) \, ,$$

$$H_2 \doteq \frac{1}{2}(N_1 N_2 (N_3 - N_4) + N_3 N_4 (N_1 - N_2)), \qquad (4.47)$$

$$H_3 \doteq \frac{1}{2}(N_2 N_4 (N_1 - N_3) - N_1 N_3 (N_2 - N_4)), \qquad (4.48)$$

and the analogous $\hat{H}_\kappa$ obtained from the H_κ once more replacing N_j with $(N_j - 1)$, provides us with the Cartan-Weyl realization of the two $su(4)$'s :

$$[\mathbf{H}, E_\kappa] = \mathbf{\Gamma}^{(\kappa)} E_\kappa \quad ; \quad [E_\kappa, E_{\kappa'}] = \mathcal{N}_{\kappa\kappa'} E_{\kappa+\kappa'} \quad ;$$

$$[H_i, H_j] = 0 \quad ; \quad [E_\kappa, E_{-\kappa}] = \mathbf{\Gamma}^{(\kappa)} \cdot \mathbf{H} \quad ; \qquad (4.49)$$

where $\mathbf{H} \equiv |H_1 H_2 H_3\rangle$, and both the vectors $\mathbf{\Gamma}^{(\kappa)}$ and the matrix $\mathcal{N}_{\kappa\kappa'}$ are straightforwardly obtained from the definitions by explicit computation.

Similarly, suitably renaming the fifteen operators M and P as:

$$\begin{aligned}
G_1 &\doteq {}^3_4 M_2^1 \quad ; \quad G_2 \doteq {}^4_3 M_2^1 \quad ; \quad G_3 \doteq {}^1_2 M_4^3 \quad ; \\
G_4 &\doteq {}^2_1 M_4^3 \quad ; \quad G_5 \doteq {}^1_4 M_3^2 \quad ; \quad G_6 \doteq {}^4_1 M_3^2 \quad ; \\
G_7 &\doteq {}^2_4 M_3^1 \quad ; \quad G_8 \doteq {}^4_2 M_3^1 \quad ; \quad G_9 \doteq {}^1_3 M_4^2 \quad ; \\
G_{10} &\doteq {}^3_1 M_4^2 \quad ; \quad G_{11} \doteq {}^2_3 M_4^1 \quad ; \quad G_{12} \doteq {}^3_2 M_4^1 \quad ; \\
G_{13} &\doteq {}^1_2 P_4^3 \quad ; \quad G_{14} \doteq {}^1_2 P_3^4 \quad ; \quad G_{15} \doteq {}^1_3 P_4^2 \quad ;
\end{aligned} \qquad (4.50)$$

and defining moreover the five Cartan operators

$$J_1 \doteq \frac{1}{\sqrt{2}}(N_1 N_2 (1 - N_3 - N_4) - N_3 N_4 (1 - N_2 - N_3)),$$

$$J_2 \doteq \frac{1}{\sqrt{2}}(N_1 N_3 (1 - N_2 - N_4) - N_2 N_4 (1 - N_1 - N_3)),$$

$$J_3 \doteq \frac{1}{\sqrt{2}}(N_1 N_4 (1 - N_2 - N_3) - N_2 N_3 (1 - N_1 - N_4)), \qquad (4.51)$$

$$J_4 \doteq \frac{1}{\sqrt{3}}(2(N_1 - N_2)(N_3 - N_4) + (N_1 - N_4)(N_2 - N_3)),$$

$$J_5 \doteq (N_1 - N_4)(N_2 - N_3),$$

we obtain, also for $su(6)$ the standard Cartan-Weyl form

$$[\mathbf{J}, G_\kappa] = \mathbf{\Omega}^{(\kappa)} G_\kappa \quad ; \quad [H_i, H_j] = 0 \quad ;$$

$$[G_\kappa, G_{\kappa'}] = \mathcal{M}_{\kappa\kappa'} G_{\kappa+\kappa'} \quad \text{with} \quad \mathbf{\Omega}^{(\kappa)} + \mathbf{\Omega}^{(\kappa')} = \mathbf{\Omega}^{(\kappa+\kappa')} \quad ; \qquad (4.52)$$

$$[G_\kappa, G_{-\kappa}] = \mathbf{\Omega}^{(\kappa)} \cdot \mathbf{J} \quad ; \quad G_{-\kappa} = G_\kappa^\dagger \quad ,$$

where $\mathbf{J} \equiv |J_1 J_2 J_3 J_4 J_5\rangle$ together with the vectors $\mathbf{\Omega}^\kappa$ and the matrix $\mathcal{M}$ completely define the algebra structure. The vectors $\mathbf{\Gamma}^{(\kappa)}$ and $\mathbf{\Omega}^\kappa$ as well as the matrix $\mathcal{N}_{\kappa\kappa'}$ are explicitly given in appendix D.

With these identifications, we can rewrite the Hamiltonian (4.37) in the form

$$\mathcal{H}_{\mathcal{D}} = \mathcal{H}_{u(1)} \oplus \mathcal{H}^{(1)}_{su(4)} \oplus \mathcal{H}^{(2)}_{su(4)} \oplus \mathcal{H}_{su(6)} \quad , \tag{4.53}$$

where (see equation (4.41))

$$\mathcal{H}_{u(1)} = \bigoplus_{\ell=0}^{4} \mathcal{H}^{(\ell)}_{u(1)} \quad , \quad \mathcal{H}^{(\ell)}_{u(1)} \equiv X^{(\ell)} C_\ell \quad , \tag{4.54}$$

One finds:

$$X^{(0)} = \bar{C} \ ; \ X^{(1)} = \frac{1}{4}(\varepsilon_1 + \varepsilon_2) \ ; \ X^{(2)} = \frac{1}{6}V \ ; \ X^{(3)} = 0 = X^{(4)} \ , \tag{4.55}$$

$$\mathcal{H}^{(1)}_{su(4)} = \sum_{k=1}^{3} h_k H_k + \sum_{i=1}^{2} (g_i E_i + c_i E_{i+3} + \text{h.c.}) \quad , \tag{4.56}$$

$$\mathcal{H}_{su(6)} = \sum_{k=1}^{5} \tilde{h}_k J_k + \sum_{i=1}^{2} \sum_{k=2i-1}^{2i} (g_i G_k + c_i G_{k+6} + \text{h.c.}) \quad , \tag{4.57}$$

$$\tag{4.58}$$

with

$$g_1 = t \ , \ g_2 = 0 \ , \ h_1 = \frac{1}{4}(\varepsilon_1 + \varepsilon_2 + 2V) \ , \ h_2 = h_3 = \frac{1}{4}(\varepsilon_1 - \varepsilon_2) \ ,$$

$$\tilde{h}_\kappa = 2\sqrt{2}\, h_\kappa \left(V \mapsto V/2 \right) \ , \ \kappa = 1, 2, 3 \ ; \ \tilde{h}_4 = \frac{1}{2\sqrt{3}}V \ ; \ \tilde{h}_5 = \frac{1}{2}V \quad ,$$

whereas $\mathcal{H}^{(2)}_{su(4)}$ is obtained from $\mathcal{H}^{(1)}_{su(4)}$ by replacing in it "hatted" operators and setting $V = 0$.

Last step to be performed in order to find the spectrum of $\mathcal{H}_{\mathcal{D}}$ is the (independent) diagonalization of the three hamiltonians $\mathcal{H}^{(1)}_{su(4)}$, $\mathcal{H}^{(2)}_{su(4)}$, and $\mathcal{H}_{su(6)}$. This is done — as customary — by a generic inner automorphism in $\mathcal{A}_{\mathcal{D}}$ (generalized Bogolubov transformation), with the procedure shown in section(1.3.2), which is valid for any Lie algebra.

Such a procedure, if one aims to obtaining only the eigenvalues of the hamiltonian, simplifies to either one of the following schemes:

1. if the fundamental faithful representation for each dynamical algebra is available, one simply writes the hamiltonian corresponding to $su(n)(n = 4, \bar{4}, 6)$ as a matrix of rank n, and the spectrum of $\mathcal{H}_{su(n)}$ is simply given by the eigenvalues $\{\omega_\kappa | \kappa = 1, \ldots, n\}$ of such matrix.

2. since the complete set of Casimir operators $\{\Gamma_\ell(\{H_i; E_{\pm\kappa}\})| \; \ell = 2, 3, 4\}$ for $su(4)$ (and obvious analogous for $su(\tilde{4})$, with $\tilde{H}_i$ and $\tilde{E}_{\pm\kappa}$ replacing H_i and $E_{\pm\kappa}$), or $\{\Gamma_\ell(\{J_i; G_{\pm\kappa}\})| \; \ell = 2, \ldots, 6\}$ for $su(6)$, where Γ_ℓ is multilinear of order ℓ in the operators, is known [60] , one can write directly the secular polynomial for $\mathcal{H}_{su(n)}$ as $\omega^n + \sum_{k=0}^{n-2} \gamma_{n-k}\, \omega^k = 0$. Here the coefficients γ_ℓ are equal to Γ_ℓ in which the operatorial arguments are replaced by the coefficient they have in $\mathcal{H}_{su(n)}$ [32].

Of course the complete solution of the problem would still require the determination in a self-consistent or variational way of the two mean-field parameter c_1 and c_2. It is worth pointing out here that the complete knowledge of the set of rotation parameters $\{\tilde{\phi}_\alpha\}$ straightforwardly leads to the evaluation of the expectation value for any operator in the following way:

$$< \hat{O} >= \frac{\text{Tr}\{\hat{O}\; e^{-\beta\mathcal{H}}\}}{\text{Tr}\{e^{-\beta\mathcal{H}}\}} = \frac{\text{Tr}\{\exp\left(\text{ad}Z(\{\tilde{\phi}_\alpha\})\right)(\hat{O})e^{-\beta\mathcal{H}_d}\}}{\text{Tr}\{e^{-\beta\mathcal{H}_d}\}} \quad . \tag{4.59}$$

From (4.59), both the free-energy – to be minimized with respect to c_1 and c_2 if the variational procedure is adopted – and the expectation value of the operators entering the self-consistency equations can be directly evaluated.

Conclusions and outlook

Motivated by the fact that the fermi-linearized conventional BCS-model is super-symmetric and exhibits spontaneous supersymmetry (SUSY)- breaking at the super-conductive critical temperature, we have investigated the possibility of identifying high-T_c phase transition with supersymmetry and its breaking.

It has been shown that the cluster fermi-linearized Hubbard model, as well as of its supersymmetric generalizations, exhibit the existence of a superconductive-magnetic phase whose appearance is associated with SUSY-breaking, and that the lattices supporting the supersymmetric charges are similar to those of two dimensional planes of Cu and O atoms in high-T_C compounds.

We have presented the first results obtained from the analysis within the scheme based on a Banach-Grassmann algebra, of the extended Hubbard model, which seems to be more appropriate to describe high-T_C superconductors than the Hubbard model. The existence of a phase with non-zero pairing has been demonstrated and a first numerical analysis of a special case (with vanishing pairing) is given. A systematic investigation of the general case will be now pursuited, in order to overcome the numerical problems arising from the high non-linearity of the involved equations.

The use of the Clifford fermi-linearization is more recent and few results have been obtained. However, the results obtained in the simplest case corresponding to the Falicov-Kimball model seem very promising and more efforts will be now devoted to numerical analysis. Work is in progress in order both to provide a complete phase space at $T = 0$ and to discuss the $T \neq 0$ behavior of the physical quantities.

Another possible development, which have not been mentioned during this thesis but seems to be very interesting, is the possibility to bridge Hubbard-like hamiltonians to phenomenological field theories, such as Chern-Simons theories, and therefore possibly to anyons.

We have seen that the identification of the SGA allows one to easily construct the generalized coherent states, which are parametrized by the points of a complex

manifold $\mathcal{M}$. For semisimple Lie (super)algebras this manifold is symplectic and can be viewed as a classical phase space for the dynamical system in question.

Let us introduce in $\mathcal{M}$ an atlas of local coordinate system $\{z, \bar{z}\}$. Since the time evolution operator maps a coherent state into another one, all the dynamical problem is reduced to the determination of a path in the coherent states manifold, and the system is described by a state

$$| \psi(t) >= e^{i\alpha(t)}| z(t) >$$

at any time t. The phase factor of $| \psi(t) >$ is given by

$$\alpha(t) = - \int_0^t h(z(\tau), \bar{z}(\tau))d\tau + \mathrm{Im} \int_0^{z(t)} \frac{\partial K}{\partial z} dz \quad ,$$

where $h(z, \bar{z}) =< z| \mathcal{H} |z >$, $\mathcal{H}$ denoting the hamiltonian operator, and $K \equiv K(z, \bar{z})$ is the so-called Kähler potential of $\mathcal{M}$, from which the metric of the manifold can be obtained. The second term in the phase is geometrical and can be viewed as a Berry's phase [12].

The adiabatic (Born-Oppenheimer) approximation is a possible treatment for systems described in terms of two typical sets of degrees of freedom which couple each other. One assumes that the separation of degrees of freedom could be realized from the onset and gets the effective hamiltonian (action) for a slow degree of freedom by "integrating out" fast variables at the first stage.

As to the adiabatic approximation, it has been found by Berry that the geometrical phase universally appears in the wave function in addition to the usual dynamical phase when the system hamiltonian changes adiabatically. This specific phase has been known to have profound effects on typical quantum phenomena covering a wide range of quantum systems. There has appeared much work related to this subject in the last years [30].

Problems such as the low-lying collective states in nuclei, where the adiabatic assumption must be removed, has stimulated the construction of frameworks which enable to derive Berry's phase beyond the adiabatic approximation [5, 45]. One possible way is to adopt the time-dependent variational principle (TDVP) [48], using the generalized coherent states as trial functions.

In [28], the analysis of dynamical effects on the geometric phase for the Two-level model has been carried out. Work is in progress along these lines with the Hubbard model [23].

The same considerations can be repeated for supercoherent states on supermanifolds. If $H = \{Q, Q^\dagger\}$ is a supersymmetric hamiltonian, the effective action

depending in this case on the local supercoherent states contains terms of the form $\int \prod_{<ij>} d\varphi_{ij} \sin(\varphi_{ij})$ where φ_{ij} is the phase difference between ϑ_i and ϑ_j. Globally, such terms give a nonvanishing contribution to the action only for closed loops in Λ, representing namely linking numbers: written in differential form over the supermanifold, the effective action derived from these hamiltonians may contain topological terms like Chern-Simons action.

Appendix A

Lie groups and algebras

A.1   Elements of group theory

An abstract set $G = \{g_1, g_2, \ldots\}$ is called a group if

1. $\forall g_1, g_2 \in G$, an associative product $g_1 g_2$ is defined [1]

2. $\exists e \in G$ such that $eg = ge = g$, $\forall g \in G$

3. $\forall g \in G$, $\exists g^{-1}$ such that $gg^{-1} = g^{-1}g = e$.

If the product is also commutative, G is *abelian*. A group with a finite number of elements is said to be *finite*.

One often encounters groups which, apart from the algebraic operations, are also endowed with a natural topology. A group is called a *topological* group if it has a topology in which the elements $g_1 g_2$ and g^{-1} are continous functions of (g_1, g_2) and g, respectively.

An important subclass of topological groups are the so-called *parametric* groups, whose elements can be parametrized (at least locally) by some systems of real parameters, i.e

$$g = g(\mathrm{t}) \equiv g(\tau_1, \ldots, \tau_n) \tag{A.1}$$

in such a way that the function $\mathrm{f}(\mathrm{t}_1, \mathrm{t}_2)$ defined by

$$g_1 g_2^{-1} = g(\mathrm{t}_1) g(\mathrm{t}_2^{-1}) = g(\mathrm{f}(\mathrm{t}_1, \mathrm{t}_2)) \tag{A.2}$$

is a continous vector valued function of t_1 and t_2.

---

[1] Obviously, closure of the product is assumed, i.e.$g_1 g_2 \in G$

Now, we can introduce the definition of Lie group. A group G is said to be a *Lie group*, if it is a parametric and the function f defining the product law is real-analytic.[2] Therefore, we can equivalently say that a Lie group is an analytic manifold, on which the group operation is analytic.

A.2   Lie algebras

Since a Lie group is an analytic manifold, it makes sense to consider the tangent space to that manifold, in particular, at the identity of the group. The union of all tangents to the manifold at e results in a linear space X of dimension n,[3] called the *Lie algebra* of G

In general, a *Lie algebra* $\mathcal{G}$ is defined as a vector space over a field F on which a product $[\ ,\ ]$, called the *Lie bracket*, satisfies the following properties:

1. $[X_i, X_j] = -[X_j, X_i]$ (anticommutativity)

2. $[\lambda X_i + \mu X_j, X_k] = \lambda[X_i, X_k] + \mu[X_i, X_k]$ (linearity)

3. $[X_i, [X_j, X_k]] + [X_k, [X_i, X_j]] + [X_j, [X_k, X_i]]$ (Jacobi identity)

If $F = \mathbb{R}, \mathbb{C}$, we say that $\mathcal{G}$ is a real, respectively, complex Lie algebra. If $\mathcal{G}$ is the tangent space X, the Lie bracket is the usual commutator, which uniquely defines multiplication in a neighborood of the corresponding group G. Therefore a Lie group G is assigned to every Lie algebra $\mathcal{G}$.

If $\{X_i\}$ is a basis of $\mathcal{G}$, then we have

$$[X_i,\ X_j] = c_{ij}^k\, X_k. \tag{A.3}$$

The set of coefficients c_{ij}^k are called the *structure constants*. From the properties of the Lie bracket, they satisfy

$$c_{ij}^m c_{mk}^n + c_{jk}^m c_{mi}^n + c_{ki}^m c_{mj}^n = 0 \tag{A.4}$$
$$c_{ij}^k = -c_{ji}^k. \tag{A.5}$$

Let us list below some algebraic fundamentals to be commonly used.

- $\mathcal{G}'$ is a *subalgebra*, if $\mathcal{G}' \subset \mathcal{G}$ and $\mathcal{G}'$ itself is a Lie algebra.

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[2] A function is said to be real-analytic if its expressible as a local power series in the neighborood of each point in its domain of definition

[3] n is the number of parameters in the group G

- A subalgebra $\mathcal{G}'$ is *invariant* or *ideal* if $[\mathcal{G}', \mathcal{G}] \subset \mathcal{G}'$

- The *center* of $\mathcal{G}$ is the largest ideal $\mathcal{C}$ such that $[\mathcal{G}, \mathcal{C}] = 0$. It is unique.

- $\mathcal{G}$ is said to be *abelian*, if $[X, Y] = 0$ for each $X, Y \in \mathcal{G}$

- $\mathcal{G}$ is said to be *simple*, if it has no invariant subalgebras besides $\mathcal{G}$ itself and $\{0\}$.

- $\mathcal{G}$ is said to be *semisimple* if it does not contain an invariant abelian subalgebra.

A *representation* is a mapping D of the Lie algebra elements to a set of matrices which preserves the Lie bracket, i.e. if $[X, Y] = Z$ then $[D(X), D(Y)] = D(Z)$. An important representation is the so-called *adjoint representation* ad_X defined by

$$\mathrm{ad}_X : \mathcal{G} \to \mathcal{G} \quad \text{such that} \quad Y \to [X, Y]. \tag{A.6}$$

where $\mathcal{G}$ itself is the vector space of the representation.

Because of the direct relations between Lie algebras and Lie groups, these definitions can be straightforwardly transferred, correspondingly.

Let $\{\mathcal{G}_i \mid i = 1, \ldots, s\}$ be a set of Lie algebras with bases $\{X_j^{(i)} \mid j = 1, \ldots, m\}$, then the *direct sum* of these Lie algebras is that linear space which is spanned by the $X_j^{(i)}$ as the composition; thus

$$\mathcal{G} = \mathcal{G}_1 \oplus \ldots \oplus \mathcal{G}_s \quad \text{with} \quad \mathcal{G}_i \cap \mathcal{G}_j = \{0\} \quad \text{for} \quad i, j = 1, \ldots, s; \; i \neq j. \tag{A.7}$$

If a Lie algebra $\mathcal{G}$ of a Lie group G is a direct sum of several algebras, then G can be represented locally as the outer *direct product*

$$G = G_1 \otimes \ldots \otimes G_s. \tag{A.8}$$

An important question arising in all applications is whether there are certain operators which commute with all the generators of a Lie algebra. In fact, this is the case, and Racah ([65]) has shown that for every semisimple Lie algebra of rank r, there exists just r independent such operators, called *Casimir invariants*, the eigenvalues of which completely specify the irreducible representations of semisimple Lie algebras.

We summarize the principal *classical* algebras in the following table:

Algebra	Constraint	Dimension	Cartan [4]
$sl(n)$	$\mathrm{Tr}\, X = 0$	$n^2 - 1$	A_{n-1}
$so(n)$	$X^t + X = 0 \;,\; \mathrm{Tr} X = 0$	$\frac{n(n-1)}{2}$	$\begin{cases} B_{\frac{n-1}{2}} & n \text{ odd} \\ D_{\frac{n}{2}} & n \text{ even} \end{cases}$
$sp(n)$	$\begin{pmatrix} \alpha_1 & \alpha_2 \\ \alpha_3 & -\alpha_1^t \end{pmatrix},\quad \alpha_2^t = \alpha_2 \;,\; \alpha_3^t = \alpha_3$	$n(2n+1)$	C_n

Appendix B

Superalgebras and Supersymmetry

B.1 Grassmann algebras

Let $\Lambda_N = \{\xi^a \ , \ a = 1, \ldots, N\}$ be a set of generators for an algebra, which anticommute:

$$\xi^a \xi^b = -\xi^b \xi^a \quad , \quad (\xi^a)^2 = 0 \quad \forall a, b \quad . \tag{B.1}$$

The algebra Λ_N is called a *Grassmann algebra*. The elements

$$\mathbb{I}, \xi^a, \xi^{a_1} \xi^{a_2}, \ldots, \xi^1 \xi^2 \ldots \xi^N \quad , \tag{B.2}$$

where the indices in each product are all different, form a basis for Λ_N with 2^N elements. Under addition as well as multiplication by a complex number, the elements of Λ_N form a linear vector space of dimension 2^N.

B.2 Lie superalgebras

A *Lie superalgebra* [1] is a $\mathbb{Z}_2$-graded vector space $\mathcal{A}$ over $\mathbb{C}$, which is the set union of of two vector subspaces $\mathcal{A}_0$ and $\mathcal{A}_1$: $\mathcal{A} = \mathcal{A}_0 \cup \mathcal{A}_1$.[2] We call Bose the even, or grade 0 elements and Fermi the odd, or grade 1 elements. $\mathcal{A}$ is endowed with a binary operation, called the super-Lie bracket, obeying the following properties:

---

[1]The term graded Lie algebra is often encountered, but since ordinary Lie algebras can also be graded, confusion can arise

[2]$\mathcal{A}_0 \cap \mathcal{A}_1 = \{0\}$

- bilinear : $[A, B] = -(-1)^{ab}[B, A] \in \mathcal{A}_{a+b}$

- super-Jacobi : $(-1)^{ac}[A, [B, C]] + (-1)^{ba}[B, [C, A]] + (-1)^{cb}[C, [A, B]] = 0$

where we denoted $a, b, c, \ldots$ the grades of the elements A, B, C: if $A \in \mathcal{G}_\alpha$, $\alpha \in \mathbb{Z}_2$, then $a = \alpha$.

A Lie superalgebra $\mathcal{A}$ is *simple* if it has no nontrivial ideals. Simple finite-dimensional superalgebras over $\mathbb{C}$ are now fully classified [42]. There are eight infinite families $sl(m|n), osp(m|n), P(n), Q(n), W(n), S(n+2), \tilde{S}(n+2), H(n+3)$, a continuum $D(2|1; \alpha)$ of 17-dimensional exceptional superalgebras, and one exceptional superalgebra each in dimensions $31(G(3))$ and $40(F(4))$.

The m generators $\{B_i$, $i = 1, \ldots, m\} \in \mathcal{A}_0$ define a Lie algebra $\mathcal{B}$ while the n generators $\{F_\alpha$, $\alpha = 1, \ldots, n\} \in \mathcal{A}_1$ are tensor operators corresponding to an n-dimensional representation $\mathcal{F}$ of $\mathcal{B}$.

The commutation (anticommutation) relations are given by

$$[\, B_m,\ B_n\,] = b^p_{mn}\, B_p \ , \tag{B.3}$$

$$[\, F_\alpha,\ B_m\,] = c^\beta_{\alpha m}\, F_\beta \ , \tag{B.4}$$

$$\{\, F_\alpha,\ F_\beta\} = f^m_{\alpha\beta}\, B_m \ , \tag{B.5}$$

where $\{b^p_{mn}, c^\beta_{\alpha m}, f^m_{\alpha\beta}\}$ are the structure constants of $\mathcal{A}$.

If the representation $\mathcal{F} = \{F_\alpha\}$ is completely reducible, one gets the *classical superalgebras*, otherwise one gets the *Cartan superalgebras* defined using fermi-dirac creation and annihilation operators.

In general, the bose sector $\mathcal{B}$ will not be simple but will contain a paiece that shuffles only the fermions, a piece that shuffles only the bosons and a piece that shuffles the bosons among themselves and the fermions among themselves. For example

$$gl(m|n)_0 = gl(m) + gl(n) \ , \tag{B.6}$$

$$sl(m|n)_0 = sl(m) + sl(n) + u(1) \ , m \neq n \ , \tag{B.7}$$

which have dimensions $m^2 + n^2$, $m^2 + n^2 - 1$ respectively. The dimensions of the corresponding Fermi parts are then $2mn$.

B.3   Supersymmetry

The notion of *Supersymmetry* (SS) was introduced by Wess and Zumino [76] in 1973 to provide the possibility to eliminate the quadratic divergences in one- and higher-loop orders associated with scalar fields masses. In that case, the SS has the effect

to couple fermions and bosons and the divergences have two sources with opposite sign coming from scalars and fermion loops so that they can be eliminated. In a more general setting, following Wytten [78], we have the following scheme.

Let $\mathcal{A}$ be a superalgebra. Then a quantum dynamical system defined by the hamiltonian $\mathcal{H} \in \mathcal{B}(\mathcal{A})$ is said to be supersymmetric if it exists $Q \in \mathcal{F}(\mathcal{A})$, such that

$$\mathcal{H} = \{ Q, Q^\dagger \} \quad , \quad Q^2 = {Q^\dagger}^2 = 0 \quad . \tag{B.8}$$

Q is called the conserved, supersymmetric charge ($[H, Q] = 0$) and excited states are fermi-bose degenerate, since $Q, Q^\dagger$ project from one to the other. Therefore Q changes the statistics of the states, and since spin is related to the behavior under spatial rotation, SS is in some sense a space-time symmetry.

If $Q| \Omega >= Q^\dagger| \Omega >= 0$, $| \Omega >$ being the vacuum, the dynamical system generated by Q is supersymmetric, otherwise the supersymmetry is said to be *spontaneously broken.*

From (B.8), for any state $|\psi >$, given that Q is hermitean, we have

$$< \psi \mid \mathcal{H} \mid \psi >= \parallel Q \mid \psi > \parallel^2 \geq 0 \tag{B.9}$$

and energy is semi-positive definite. Thus, any zero energy state is guaranteed to be a possible ground state. On the other hand, a state is supersymmetric if it annihilated by Q, and equation (B.9) implies that any state of zero energy is supersymmetric and viceversa. Therefore, to decide whether a system is supersymmetric, or breaks supersimmetry spontaneously, we just have to find out whether it has zero energy states.

Appendix C

Coherent states

Coherent states (CS) have been first introduced in quantum optics by Glauber [33] as the states of minimum uncertainty for the harmonic oscillator. Glauber's CS preservetheir shape during time evolution. After the work of Glauber several attempts have been made to generalize the concept of CS to system with a larger dynamical group [9].

We briefly review the fundamental definitions and properties of the theory of *generalized coherent states*(GCS) [61],[66].

Let $\mathcal{G}$ be the dynamical algebra of our model, G an element of the class of the corresponding Lie groups [1] and T a unitary representation (UIR) of G on a Hilbert space V.

We now assume there exists a fixed cyclic vector $|\phi_0 >\in V$ and call H the set of elements $h \in G$ such that

$$T(h)|\phi_0 >= e^{i\alpha(h)}|\phi_0 > \quad , \quad \alpha : H \to \mathbb{R} \quad . \tag{C.1}$$

$H \subset G$ will be called the *isotropy subgroup* of $|\phi_0 >$ and $e^{i\alpha}$ is a unitary character of H. Let $M = G/H$ be the left coset of G with respect to H. We can define the coherent states of $\mathcal{G}$ by means of a mapping from M to V, which associates to each $x \in M$, defined by the composition $g = x \cdot h$, with $g \in G$ and $h \in H$, the state (up to a phase factor)

$$|x >= T(x)|\phi_0 > \quad . \tag{C.2}$$

Thus the coherent states are represented by the point of a manifold M, on which G acts transitively by means of the left translation $\circ : G \times M \to M$ defined by

$$g \circ x = \pi(g \cdot \pi^{-1}(x)) \quad , \quad \forall g \in G \,, \, x \in M \quad , \tag{C.3}$$

---

[1] To a given group correspond a unique Lie algebra. However, the converse is not true.

π being the natural projection of G on M. Therefore G is a fibre bundle over M as base space relative to π and the fibre of the bundle is H.

The transitivity of M with respect to G reflects an important property of the system of states just defined: the action of the dynamical group G maps coeherent states into other coherent states. Another important properties are the resolution of the identity and the (over)completeness of the system, of fundamental importance in the coherent states representation of the Feynman path integral. Let $d\mu(x)$, $\forall x \in M$ be a G-invariant measure on the manifold M, then an arbitrary state $|\psi > \in V$ can in fact be expanded in terms of coherent states

$$|\psi >= \frac{1}{c} \int d\mu(x)|x > \underbrace{< x \mid \psi >}_{\equiv \psi(x)} \qquad (C.4)$$

where the function $\psi(x)$ is a solution of the integral equation

$$\psi(x) = \frac{1}{c} \int d\mu(y) < x \mid y > \psi(y) \quad . \qquad (C.5)$$

For a real semisimple Lie algebra, the algebra of the isotropy subgroup H is just the Cartan subalgebra if the representation is non degenerate, but can be larger if the representation is degenerate.

For Lie superalgebras, coherent states may be defined as for usual Lie algebras [59]. The left coset space M will be a supermanifold (that is a manifold with even and odd coordinates) and therefore the integrations in (C.4) and (C.5) must be intended as an ordinary integration for what concerns even variables, and as a Berezin integration for what concerns odd variables.

Appendix D

Technical remarks on su(4) and su(6)

We give the explicit coefficients $\{\Gamma^{(\kappa)}, \Omega^{(\kappa)}, \mathcal{N}\}$ entering in the Cartan-Weyl form of the algebras $su(4)$ and $su(6)$ defined in (4.49) and (4.52). $\mathcal{M}$ is too big, but the commutators can be easily deduced from the considerations about $su(6)$ at the end of the appendix.

From the following matrix $\mathbf{A}$ defined as

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 0 & 0 & 1 \\ 1 & -1 & 0 & 1 & -1 & 0 \end{pmatrix} , \tag{D.1}$$

we can derive the vector $\Gamma^{(k)}$ writing $\Gamma_i^{(k)} = A_{ik}$, while from the matrix

$$\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 & -1 \\ 1 & -1 & 0 & -1 & -1 & 0 \end{pmatrix} , \tag{D.2}$$

we deduce the matrix $\mathcal{N}$ as $\mathcal{N}_{ij} = B_{i,i+j}$. The other coefficients of $\mathcal{N}$ are straightforwardly obtained using the properties $\mathcal{N}_{\alpha\beta} = -\mathcal{N}_{\beta\alpha} = -\mathcal{N}_{-\alpha,-\beta} = \mathcal{N}_{-\beta,-\alpha}$.

In an analogous way, for the Lie algebra $su(6)$, we define the matrix $\tilde{A}$

$$
\tilde{A} = \frac{1}{2}
\begin{pmatrix}
0 & \sqrt{2} & \sqrt{2} & \sqrt{3} & -1 \\
0 & \sqrt{2} & \sqrt{2} & -\sqrt{3} & 1 \\
0 & \sqrt{2} & -\sqrt{2} & \sqrt{3} & -1 \\
0 & \sqrt{2} & -\sqrt{2} & -\sqrt{3} & 1 \\
\sqrt{2} & -\sqrt{2} & 0 & 0 & 2 \\
\sqrt{2} & -\sqrt{2} & 0 & 0 & -2 \\
\sqrt{2} & 0 & \sqrt{2} & \sqrt{3} & 1 \\
\sqrt{2} & 0 & \sqrt{2} & -\sqrt{3} & -1 \\
\sqrt{2} & 0 & -\sqrt{2} & \sqrt{3} & 1 \\
\sqrt{2} & 0 & -\sqrt{2} & -\sqrt{3} & -1 \\
\sqrt{2} & \sqrt{2} & 0 & 0 & 2 \\
\sqrt{2} & \sqrt{2} & 0 & 0 & -2 \\
0 & 2\sqrt{2} & 0 & 0 & 0 \\
0 & 0 & 2\sqrt{2} & 0 & 0 \\
2\sqrt{2} & 0 & 0 & 0 & 0
\end{pmatrix}
. \tag{D.3}
$$

The vector $\Omega^{(k)}$ is then given by $\Omega_i^{(k)} = \tilde{A}_{ki}$.

Let us conclude giving a possible representation for the algebra $su(6)$. Even if the commutation relations of the operators $\{{}^{\gamma}_{\delta}M_{\alpha}^{\beta} , {}^{\gamma}_{\delta}P_{\alpha}^{\beta}\}$ given in (4.44),(4.45), (4.46) are not transparent, the $su(6)$ structure is readily recognized defining a set of six fictitious fermions $\{c_{\alpha}, c_{\alpha}^{\dagger}\}$ and the associated 15 bilinears F_{α}^{β}, which automatically satisfy the $su(6)$ algebra

$$
[F_{\alpha}^{\beta} , F_{\gamma}^{\delta}] = \delta_{\beta\gamma}F_{\alpha}^{\delta} - \delta_{\alpha\delta}F_{\gamma}^{\beta} \quad . \tag{D.4}
$$

The identification between the two set of operators is then:

$$
\begin{array}{lll}
F_2^1 = -P_2 & F_3^2 = M_3 & F_5^3 = -M_{-12} \\
F_3^1 = M_1 & F_4^2 = -M_9 & F_6^3 = -P_{-1} \\
F_4^1 = M_7 & F_5^2 = M_{-8} & F_5^4 = -P_{-3} \\
F_5^1 = M_{-10} & F_6^2 = M_{-2} & F_6^4 = -M_{-11} \\
F_6^1 = M_{-4} & F_4^3 = M_5 & F_6^5 = M_6 \quad .
\end{array} \tag{D.5}
$$

Obviously, this is only a faithful representation and only operations (like adjoint actions) involving commutators may be done.

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