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Orthogonality constraints and entropy in the SO(5)-theory of high T_c-superconductivity

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Abstract. Zhang has put forward the idea that high-temperature-superconductors can be described in the framework of an SO(5)-symmetric theory in which the three components of the antiferromagnetic order-parameter and the two components of the two-particle condensate form a five-component order-parameter with SO(5) symmetry. Interactions small in comparison to this strong interaction introduce anisotropies into the SO(5)-space and determine whether it is favorable for the system to be superconducting or antiferromagnetic. Here the view is expressed that Zhang's derivation of the effective interaction V_{eff} based on his Hamiltonian H_{a} is not correct. However, the orthogonality constraints introduced several pages after this "derivation" give the key to an effective interaction very similar to that given by Zhang. It is shown that the orthogonality constraints are not rigorous constraints, but they maximize the entropy at finite temperature. If the interaction drives the ground-state to the largest possible eigenvalues of the operators under consideration (antiferromagnetic ordering, superconducting condensate, etc.), then the orthogonality constraints are obeyed by the ground-state, too.

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1 Introduction

In a recent paper [1] Zhang has proposed the idea that the components of the electron-pair condensate and those of the antiferromagnetic order-parameter form a five-component order parameter in an approximately SO(5)-invariant theory. Anisotropies small in comparison to the SO(5)-invariant interaction break this symmetry. They depend in particular on the chemical potential and thus on doping. This allows him to describe the transition from antiferromagnetism in the half-filled system to superconductivity under moderately weak doping.

This phenomenological picture has been tested by numerical calculations for small Hubbard-systems [2,3] and t-J-models [3,4], for which good agreement with the predictions from Zhang's theory are obtained. It has also been shown that spin-ladders observe SO(5)-symmetry [5,6] or even SO(8)-symmetry [7].

Returning to higher-dimensional systems, it is pointed out here that Zhang's derivation of the effective interaction V_{eff} based on his Hamiltonian H_{a} seems to be not correct. (Actually we struggled for quite a while trying to understand his derivation). However, the orthogonality constraints introduced several pages after this "derivation" give the key to an effective interaction very similar to that given by Zhang. After having established this in Section 2 it is shown in Section 3, that the entropy contains squares of these constraint terms. Thus the orthogonality constraints are not strict requirements, but their fulfillment maximizes the entropy and lowers the free energy. Finally in Section 4 it is argued, that also in the ground-state these constraints are likely to hold.

2 Effective interaction and the orthogonality constraint

Zhang introduces a five-component order-parameter n_i, $i = 1..5$. The operators associated with these components are given explicitly in the Appendix. Two components, n_1 and n_5, describe the real part and the imaginary part of the superconducting condensate, the three other components n_2, n_3, and n_4, are the three Cartesian components of the staggered magnetization. He assumes that a strong interaction which may be described by a Ginzburg-Landau interaction, leads to a symmetry breaking below a critical temperature T_{c} and has an SO(5) symmetry, thus allowing both superconducting and antiferromagnetic order. This leading interaction is a function of $\sum_i n_i^2$ only and does

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not give any preference to superconducting or antiferromagnetic order.

In addition there is a weaker interaction $H_{\rm a}$ which introduces anisotropy into the system

$$H_{\rm a} = \frac{L_{1,5}^2}{2\chi_{\rm c}} + \frac{L_{1,2}^2 + L_{1,3}^2 + L_{1,4}^2 + L_{2,5}^2 + L_{3,5}^2 + L_{4,5}^2}{2\chi_\pi} + \frac{L_{2,3}^2 + L_{2,4}^2 + L_{3,4}^2}{2\chi_{\rm s}} - \frac{g}{2}(n_2^2 + n_3^2 + n_4^2) - 2\mu L_{1,5}. \tag{1}$$

The $L_{a,b}$ are operators bilinear in the electron creation and annihilation operators. They are given explicitly in Appendix A. μ is the chemical potential. The operators L obey $L_{b,a} = -L_{a,b}$ and the commutator relations

$$[L_{a,b}, L_{c,d}] = -{\rm i}\delta_{b,c}L_{a,d} + {\rm i}\delta_{a,c}L_{b,d} + {\rm i}\delta_{b,d}L_{a,c} - {\rm i}\delta_{a,d}L_{b,c} \tag{2}$$

of the orthogonal group SO(5), moreover the vector n is rotated by L,

$$[L_{a,b}, n_c] = -{\rm i}\delta_{b,c}n_a + {\rm i}\delta_{a,c}n_b. \tag{3}$$

The derivative terms of Zhang's interaction are left out here, since only the global state is investigated. The effective potential is determined as the minimum of the Hamiltonian for given order-parameter n_1, ... n_5, which Zhang normalizes to

$$\sum_i n_i^2 = 1. \tag{4}$$

Since one considers the interaction for a macroscopic system, all the components of L and n can be considered as classical quantities and the obvious minimum is obtained for $L_{1,5} = 2\mu\chi_{\rm c}$, whereas all other components of L vanish, which yields what I call $V_{\rm eff}^{\rm naiv}$

$$V_{\rm eff}^{\rm naiv}(n) = -2\mu^2\chi_{\rm c} - \frac{g}{2}(n_2^2 + n_3^2 + n_4^2). \tag{5}$$

It would mean that the only effect of the chemical potential is a lowering of the energy of the system, but it would have no effect on an anisotropy in the order-parameter space. This obviously is at variance with Zhang's claim for the effective interaction

$$V_{\rm eff}^{\rm Zhang}(n) = -2\mu^2(n_1^2 + n_5^2)[\chi_{\rm c}(n_1^2 + n_5^2) + \chi_\pi(n_2^2 + n_3^2 + n_4^2)] - \frac{g}{2}(n_2^2 + n_3^2 + n_4^2). \tag{6}$$

An indication that Zhang's Lagrangian

$$\mathcal{L}_{\rm a} = \sum_{a<b} \frac{\chi_{ab}}{2}\omega_{ab}^2 + V(n) \tag{7}$$

$$\omega_{ab} = n_a(\partial_\tau n_b - {\rm i}B_{bc}n_c) - (a \to b) \tag{8}$$

is not equivalent to $H_{\rm a}$, is obvious from the fact that in Zhang's Lagrangian the only allowed rotations are in the plain spanned by n and $\partial_\tau n - {\rm i}Bn$, whereas it does not permit a rotation around a second perpendicular plain (which exists in 5 dimensions) as it should. Thus the description by $\mathcal{L}_{\rm a}$ is incomplete.

However, several pages later he introduces the constraints

$$\epsilon_{a,b,c,d,e}n_c L_{d,e} = 0. \tag{9}$$

These constraints, (although not proven in Zhang's paper, since (8) is not granted) are the key for the effective interaction. If they are fulfilled, then one can conclude, that L is of the form

$$L_{a,b} = c_a n_b - c_b n_a. \tag{10}$$

(This can be found in the following way: If $n_1 = 1$, and all other n_i vanish, then one finds from (9) $L_{a,b} = 0$, if both $a \neq 1$ and $b \neq 1$. However $L_{a,1} = -L_{1,a} = c_a$ for $a \neq 1$ can be chosen with arbitrary c_a. Thus one obtains in this special case equation (10). The relation (10) is form-invariant under SO(5)-rotations. Thus it holds for general n_i.)

Apparently in the literature [1,8] two different rotator pictures are mixed. The first one starts from the Hamiltonian $H_{\rm a}$, which describes a rotator with nonvanishing moments of inertia (actually susceptibilities χ) for rotations in all plains. The second picture seems to consider n as a rotator with vanishing moments of inertia for rotations in plains perpendicular to n. This second picture yields immediately equation (10). However, it does not directly follow from the original (first) picture. Thus, if equation (9) or (10) is to hold, we have to find a reason for it, which will be given in Section 3.

Let us return to equation (10). It has two consequences:

(i) One can now parametrize $H_{\rm a}$ in terms of the c_i and determine the minimum as one varies the coefficients c. One finds the minimum for

$$c_2 = c_3 = c_4 = 0, \quad c_1 = \frac{2\mu n_5}{N}, \quad c_5 = -\frac{2\mu n_1}{N} \tag{11}$$

with

$$N = \frac{n_1^2 + n_5^2}{\chi_{\rm c}} + \frac{n_2^2 + n_3^2 + n_4^2}{\chi_\pi}\,. \tag{12}$$

From this one obtains the effective interaction

$$V_{\rm eff} = -2\mu^2\frac{n_1^2 + n_5^2}{N} - \frac{g}{2}(n_2^2 + n_3^2 + n_4^2). \tag{13}$$

For $\chi_{\rm c} = \chi_\pi$ it agrees with $V_{\rm eff}^{\rm Zhang}$. If $\chi_{\rm c} \neq \chi_\pi$, then the effective potentials are different (actually in first order in $\chi_{\rm c} - \chi_\pi$ there is still agreement), but many conclusions Zhang has drawn will continue to hold. After submission of this paper I was kindly informed by Zhang and Auerbach, that the effective potential equation (13) was already derived in equation (108) of Auerbach's lecture notes of the Chia Laguna Summer School [8].

(ii) The constraints imply, that out of the representations (λ_1, λ_2) the only allowed states have representations of the form $(\lambda_1, 0)$. Let me explain this shortly. The irreducible representations of SO(5) are characterized by two (non negative) numbers (λ_1, λ_2) with $\lambda_1 \geq \lambda_2 \geq 0$. The first number is the largest eigenvalue of one of the operators L, say $L_{1,2}$. Next consider the subspace of the states in this representation with this eigenvalue λ_1 for $L_{1,2}$. Then λ_2 is the largest eigenvalue of one of the operators L, that commutes with the first one, which may be $L_{3,4}$ in this subspace. Semiclassically, that is for large λ_1 and λ_2, one may replace the operators $L_{a,b}$ by their expectation values. Then the eigenvalues of the antisymmetric matrix L are $\pm \mathrm{i}\lambda_1$, $\pm \mathrm{i}\lambda_2$ and 0. If L has the form (10), then

$$\lambda_1 = \sqrt{\sum_i c_i^2 \sum_j n_j^2 - (\sum_i c_i n_i)^2}, \quad \lambda_2 = 0. \tag{14}$$

Therefore the main problem left is to understand why the orthogonality constraints should hold. This will be done in the next section.

3 Entropy as source of the orthogonality constraint

We claim that the orthogonality constraints are an effect of entropy. It will be shown that a system even without any interaction has entropic parts of the form

$$-\big(\epsilon_{a,b,c,d,e} n_c L_{d,e}\big)^2 \tag{15}$$

which make it favorable for the system to obey the orthogonality constraints. Thus (9) is not a strict constraint, but if it is fulfilled, then the entropy assumes a maximum.

3.1 Entropy of the Heisenberg antiferromagnet

First consider the Heisenberg antiferromagnet as an example, which Zhang has rightly mentioned in his paper. The Heisenberg antiferromagnet consists of two sublattices with magnetizations $\mathbf{m}_1$ and $\mathbf{m}_2$. We expand the entropy in powers of $\mathbf{m}_1^2$ and $\mathbf{m}_2^2$. Since the two sublattice-magnetizations describe the behaviour on different sublattices, the entropy is a sum of contributions on these sublattices

$$S = S_0 - c_1(\mathbf{m}_1^2 + \mathbf{m}_2^2) - c_2\big((\mathbf{m}_1^2)^2 + (\mathbf{m}_2^2)^2\big) - ... \tag{16}$$

Then denoting the homogeneous magnetization by $\mathbf{m}_0$ and the staggered magnetization by $\mathbf{m}_{q_0}$ we may write $\mathbf{m}_1 = \mathbf{m}_0 + \mathbf{m}_{q_0}$ and $\mathbf{m}_2 = \mathbf{m}_0 - \mathbf{m}_{q_0}$ and obtain the entropy

$$\begin{aligned} S = S_0 - 2c_1(\mathbf{m}_0^2 + \mathbf{m}_{q_0}^2) - 2c_2\big(\mathbf{m}_0^2 + \mathbf{m}_{q_0}^2\big)^2 \\ - 8c_2\big(\mathbf{m}_0 \cdot \mathbf{m}_{q_0}\big)^2 - ... \end{aligned} \tag{17}$$

Thus if there is no coupling in the interaction between $\mathbf{m}_0$ and $\mathbf{m}_{q_0}$, the system prefers to have the homogeneous and the staggered magnetization orthogonal to each other due to the contribution $-8c_2(\mathbf{m}_0 \cdot \mathbf{m}_{q_0})^2$ in the entropy. Remember that the entropy enters into the free energy with a minus sign ($F = E - TS$), and thus $\mathbf{m}_0 \cdot \mathbf{m}_{q_0} = 0$ will yield the minimum of the free energy. Thus there is not a strict constraint $\mathbf{m}_0 \cdot \mathbf{m}_{q_0} = 0$ for the Heisenberg antiferromagnet, but there is a term proportional to the square $(\mathbf{m}_0 \cdot \mathbf{m}_{q_0})^2$ in the free energy, which favors the constraint to be obeyed.

3.2 The entropy

It will now be shown that the entropy of the more general SO(5)-invariant system contains terms of type $(\epsilon_{a,b,c,d,e} n_c L_{d,e})^2$. We will actually enlarge the system of operators $L_{a,b}$ to those of an SO(8) (for details see in the Appendix). To determine the entropy we start from the Hamiltonian

$$H_\Omega = \sum_{a,b} \Omega_{a,b} L_{a,b}, \quad \Omega_{b,a} = -\Omega_{a,b} \tag{18}$$

where the set of our $L_{a,b}$ also includes the $n_a = L_{a,0}$. We do no longer use the normalization (4). We note, that recently a U(4)-scheme including the operators $L_{a,b}$ with $a, b = 0..5$ and $L_{6,7}$ and their sub-groups has been considered in [9] (note that SU(4) is isomorphous to SO(6)). Similar ideas are found in [10]. The Ω are introduced as Lagrange multipliers and will be adjusted to yield given expectation values of $L_{a,b}$, and the entropy will be calculated up to fourth order in L.

Ω is an eight-dimensional antisymmetric real matrix. Since the matrix is antihermitean, its eigenvalues are purely imaginary and occur pairwise. Thus the eigenvalue equation can be written

$$\sum_b \Omega_{a,b}(x_b^{(k)} \pm \mathrm{i} y_b^{(k)}) = \pm \mathrm{i}\omega^{(k)}(x_a^{(k)} \pm \mathrm{i} y_a^{(k)}) \tag{19}$$

with $k = 1..4$ and real vectors $x^{(k)}$ and $y^{(k)}$. The vectors $x^{(k)}$ and $y^{(k)}$ are orthogonal to each other. If they are normalized, then Ω may be represented

$$\Omega_{a,b} = \sum_k \omega^{(k)}(x_a^{(k)} y_b^{(k)} - x_b^{(k)} y_a^{(k)}). \tag{20}$$

Next we perform a special orthogonal transformation, so that $x^{(k)}$ and $y^{(k)}$ are oriented in appropriate directions, *e.g.* so that $x^{(1)}$, $y^{(1)}$ point in the 5- and 1- direction, $x^{(2)}$, $y^{(2)}$ in the 2- and 3-direction, $x^{(3)}$ and $y^{(3)}$ in the 0- and 7-direction and $x^{(4)}$ and $y^{(4)}$ in the 4- and 6- direction, respectively. After this special orthogonal transformation H reads

$$\begin{aligned} &H_{\mathrm{trans}} = \\ &2(\omega^{(1)} N^0_{0,1,1} + \omega^{(2)} N^0_{0,1,\sigma^z} + \omega^{(3)} N^0_{0,g,1} - \omega^{(4)} N^0_{0,g,\sigma^z}) \\ &= \sum_{k,s} (\omega^{(1)} + \omega^{(2)} s + \omega^{(3)} g(k) - \omega^{(4)} g(k) s)(c^\dagger_{k,s} c_{k,s} - \frac{1}{2}) \end{aligned} \tag{21}$$

(with $s = \pm 1$, $g(k) = \pm 1$, $g(k+q_0) = -g(k)$). Thus for momenta k and $k+q_0$ one has in total 2^4 states constructed out of four single-particle states, which may be either occupied or unoccupied and which contribute the energies $\pm\frac{1}{2}\epsilon_{s,g}$ depending on whether the state is occupied or unoccupied

$$\epsilon_{s,g} = \omega^{(1)} + \omega^{(2)}s + \omega^{(3)}g - \omega^{(4)}gs. \tag{22}$$

Then we obtain for the partition function Z

$$\ln Z = \sum \ln\left(\exp\left(\frac{1}{2}\beta\epsilon\right) + \exp\left(-\frac{1}{2}\beta\epsilon\right)\right)$$
$$= \sum\left(\ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + O(x^6)\right), \quad x = \frac{\beta\epsilon}{2}\cdot \tag{23}$$

Summation over the four states yields

$$\sum x^2 = \beta^2 \sum_i \omega^{(i)2} \tag{24}$$

$$\sum x^4 = \frac{\beta^4}{4}\left(\sum_i \omega^{(i)4} + 6\sum_{i<j}\omega^{(i)2}\omega^{(j)2} - 24\omega^{(1)}\omega^{(2)}\omega^{(3)}\omega^{(4)}\right). \tag{25}$$

Similarly we expand the entropy S

$$S = k_{\mathrm{B}}\sum\left(\ln 2 - \frac{x^2}{2} + \frac{x^4}{4} + O(x^6)\right) \tag{26}$$

and determine the expectation value of the quantity $L^{(i)}$ conjugate to $\omega^{(i)}$ (only the first component is given; the others are obtained by permutation),

$$L^{(1)} = \frac{\partial \ln Z}{2\beta\partial\omega^{(1)}} = \frac{\beta}{2}\omega^{(1)} - \frac{\beta^3}{24}\big(\omega^{(1)3} + 3\omega^{(1)}(\omega^{(2)2} + \omega^{(3)2} + \omega^{(4)2}) - 6\omega^{(2)}\omega^{(3)}\omega^{(4)}\big) + O(\omega^5) \tag{27}$$

and express $\omega^{(i)}$ in terms of $L^{(i)}$,

$$\beta\omega^{(1)} = 2L^{(1)} + \frac{2}{3}\big(L^{(1)3} + 3L^{(1)}(L^{(2)2} + L^{(3)2} + L^{(4)2}) - 6L^{(2)}L^{(3)}L^{(4)}\big) + O(L^5). \tag{28}$$

In diagonal form one has $L^{(1)} = L_{5,1}$, etc. Then S for the subspace of the electrons with momenta k and $k+q_0$ reads

$$S/k_{\mathrm{B}} = 4\ln 2 - 2\sum_i L^{(i)2} - \frac{1}{3}\left(\sum_i L^{(i)4} + 6\sum_{i<j} L^{(i)2}L^{(j)2} - 24L^{(1)}L^{(2)}L^{(3)}L^{(4)}\right) + O(L^6). \tag{29}$$

Thus we have expressed the entropy in terms of the eigenvalues $\pm\mathrm{i}L^{(i)}$ of the 8×8-matrix $(L_{a,b})$ of the expectation values $L_{a,b}$. We will express it now by the matrix-elements of L. First we have

$$\sum_i L^{(i)2} = -\frac{1}{2}\mathrm{Tr}L^2 = -\sum_{a<b} L_{a,b}^2, \tag{30}$$

$$\sum_i L^{(i)4} = \frac{1}{2}\mathrm{Tr}L^4 = \sum_{a<b} L_{a,b}^4 + 2\sum_{a,b<c} L_{a,b}^2 L_{a,c}^2 + 4\sum_{a<b,a<c<d,b\neq c,b\neq d} L_{a,c}L_{a,d}L_{b,c}L_{b,d}, \tag{31}$$

$$\sum_i L^{(i)4} + 2\sum_{i<j} L^{(i)2}L^{(j)2} = \frac{1}{4}(\mathrm{Tr}L^2)^2 = \sum_{a<b} L_{a,b}^4 + 2\sum_{a,b<c} L_{a,b}^2 L_{a,c}^2 + 2\sum_{a<b,a<c<d,b\neq c,b\neq d} L_{a,b}^2 L_{c,d}^2, \tag{32}$$

$$L^{(1)}L^{(2)}L^{(3)}L^{(4)} = \mathrm{pf}(L), \tag{33}$$

where $\mathrm{pf}(L)$ is the Pfaffian of L. In our case the indices a, b of the elements $L_{a,b}$ are numbered from 0 to 7. Then the Pfaffian (which is defined only for antisymmetric matrices) is the sum $\sum_{k=1}^{7}(-)^{k-1}L_{0,k}P_k$, where P_k is the Pfaffian of the matrix obtained from the matrix L by deleting the rows and columns with index 0 (that is the first one) and index k. One continues recursively until the Pfaffian of a matrix with no entry is left, which is defined to equal 1. (If one starts with a matrix of odd dimension, then finally one arrives at the Pfaffian of the 1×1 matrix with entry 0, since it has to be antisymmetric. This Pfaffian is defined to equal 0. Therefore the Pfaffian of a matrix of odd dimensions vanishes.) We mention that the determinant of an antisymmetric matrix equals the square of its Pfaffian. For 2×2 and 4×4 matrices the Pfaffians read

$$\mathrm{pf}\begin{pmatrix} 0 & L_{a,b} \\ -L_{a,b} & 0 \end{pmatrix} = L_{a,b} \tag{34}$$

$$p_{a,b,c,d} := \mathrm{pf}\begin{pmatrix} 0 & L_{a,b} & L_{a,c} & L_{a,d} \\ -L_{a,b} & 0 & L_{b,c} & L_{b,d} \\ -L_{a,c} & -L_{b,c} & 0 & L_{c,d} \\ -L_{a,d} & -L_{b,d} & -L_{c,d} & 0 \end{pmatrix} = L_{a,b}L_{c,d} - L_{a,c}L_{b,d} + L_{a,d}L_{b,c}. \tag{35}$$

Then we have

$$S/k_{\mathrm{B}} = 4\ln 2 + \mathrm{Tr}L^2 - \frac{1}{3}\big(\frac{3}{4}(\mathrm{Tr}L^2)^2 - \mathrm{Tr}L^4 - 24\mathrm{pf}(L)\big). \tag{36}$$

(Note that $\mathrm{Tr}L^2$ is negative). Further algebraic manipulations yield

$$-\mathrm{Tr}L^4 = -\frac{1}{2}(\mathrm{Tr}L^2)^2 + 4\sum_{a<b<c<d} p_{a,b,c,d}^2, \tag{37}$$

$$24\mathrm{pf}(L) \quad = \quad 4\sum_{a<b<c<d,\, e<f<g<h} \epsilon_{a,b,c,d,e,f,g,h}\, p_{a,b,c,d}\, p_{e,f,g,h}. \tag{38}$$

Putting all the contributions together we obtain

$$S/k_\mathrm{B} = 4\ln 2 + \mathrm{Tr}L^2 - \frac{1}{12}(\mathrm{Tr}L^2)^2 - \frac{4}{3}\sum_{0<a<b<c}\Big(p_{0,a,b,c} - \sum_{d<e<f<g} \epsilon_{a,b,c,d,e,f,g} p_{d,e,f,g}\Big)^2 + O(L^6). \tag{39}$$

This corresponds to the separation of (29) into

$$S/k_\mathrm{B} = 4\ln 2 - 2\sum_i L^{(i)2} - \frac{1}{3}\left(\sum_i L^{(i)2}\right)^2 - \frac{4}{3}\big((L^{(1)}L^{(2)} - L^{(3)}L^{(4)})^2 + (L^{(1)}L^{(3)} - L^{(2)}L^{(4)})^2 + (L^{(1)}L^{(4)} - L^{(2)}L^{(3)})^2\big) + O(L^6). \tag{40}$$

Thus the entropy consists of a completely rotational invariant contribution depending only on $\mathrm{Tr}L^2$ and a negative sum of squares of $p_{0,a,b,c} \pm p_{d,e,f,g}$. Note that the sum over d, e, f, g contains exactly one term $\pm p$. Thus a maximum of the entropy is reached, when the arguments of all the squares vanish. Provided $L_{a,b}$ vanishes if a or b equals 6 or 7 as assumed in the SO(5) theory, then out of the 35 squares 20 vanish identically, 10 have the form $\epsilon_{a,b,c,d,e} n_c L_{d,e}$, which when required to vanish are Zhang's orthogonality constraints, and 5 have the form $\epsilon_{a,b,c,d,e} L_{b,c} L_{d,e}$. One can easily see from (10), that if Zhang's orthogonality constraints are fulfilled, then also these latter quantities vanish. Thus the orthogonality constraints are not strict requirements, but their fulfillment lowers the free energy.

We mention, that the vanishing of the squares in the second line of (40) implies two types of solutions, either one $L^{(i)}$ can be different from zero and the other $L^{(j)}$ vanish, or all $|L^{(i)}|$ are equal, and the product of the four $L^{(i)}$ is positive.

At half-filling (no doping) one has $L_{1,5} = 0$. Then in the antiferromagnetic state, that is for non-vanishing components $L_{2,0}$, $L_{3,0}$, and $L_{4,0}$, but otherwise vanishing components L, only one eigenvalue $L^{(i)}$ is different from zero. As soon as one has some doping $L_{1,5}$ is different from 0. If the system is still antiferromagnetic, then more than one eigenvalue differs from zero. On the other hand, if the modes associated with $n_6 = L_{6,0}$ or $n_7 = L_{7,0}$ are massive, as assumed, then it costs energy to have all four eigenvalues $L^{(i)}$ different from zero. Then it becomes preferable to have the superconducting components $n_1 = L_{1,0}$ and $n_5 = L_{5,0}$ different from zero and to have vanishing antiferromagnetism, since then again one has only one nonvanishing eigenvalue $L^{(i)}$.

4 Limits for the ground state

The entropy argument given in the preceding section can be applied in the vicinity of the critical temperature. At low temperatures the contribution of the entropy to the free energy decreases, since it enters with the factor T. Therefore we consider separately the situation at low temperatures.

4.1 Antiferromagnet

Let us start with a simple consideration for the antiferromagnet. Assume again two sublattices with magnetization $\mathbf{m}_1$ and $\mathbf{m}_2$. Assume they are restricted by upper bounds $|\mathbf{m}_1| \le 1$, $|\mathbf{m}_2| \le 1$. Suppose now the system has a homogeneous magnetization $\mathbf{m}_0$. If now a staggered magnetization parallel to $\mathbf{m}_0$ is added, then apparently $|\mathbf{m}_{q_0}| \le 1 - |\mathbf{m}_0|$. If however the staggered magnetization is perpendicular to the homogeneous one, then one has the weaker restriction $|\mathbf{m}_{q_0}| \le \sqrt{1 - \mathbf{m}_0^2}$. Thus the antiferromagnetic interaction can act more strongly, if the staggered magnetization is perpendicular to the homogeneous one. Thus again $\mathbf{m}_0 \cdot \mathbf{m}_{q_0} = 0$ is fulfilled.

4.2 Hartree-Fock-Bogoliubov ground state

We have seen, that at low temperatures the bounds on the appropriate quantities (order-parameters) are important for the ordering of the ground-state. Therefore we will consider the bounds of the eigenvalues $\pm \mathrm{i}L^{(i)}$ of the matrix L. If for a fixed matrix Ω in (18) one takes the low temperature limit $\beta \to \infty$, then normally a pure Hartree-Fock-Bogoliubov state instead of a mixed state remains. Depending on the sign of $\epsilon_{s,g}$ the occupation number $n_{s,g}$ assumes one of its extremal values 0 and 1 in the diagonal representation H_trans (21)

$$n_{s,g} = \frac{1}{2} - \frac{1}{2}\mathrm{sign}\epsilon_{s,g}. \tag{41}$$

From this we obtain the eigenvalues $L^{(i)}$

$$L^{(1)} = \frac{1}{2}\sum_{s,g} n_{s,g} - 1 \tag{42}$$

$$L^{(2)} = \frac{1}{2}\sum_{s,g} s\, n_{s,g} \tag{43}$$

$$L^{(3)} = \frac{1}{2}\sum_{s,g} g\, n_{s,g} \tag{44}$$

$$L^{(4)} = \frac{1}{2}\sum_{s,g} sg\, n_{s,g}. \tag{45}$$

Putting now $n_{s,g} = 0$ or 1 in all combinations one finds two types of solutions for $L^{(i)}$. In the first class one $L^{(i)} = \pm 1$ and the other $L^{(j)} = 0$, whereas in the second class one has $L^{(i)} = \pm\frac{1}{2}$ for all i with the restriction for the signs, that the product of all $L^{(i)}$ is positive. One easily realizes that in all these cases the squares in the second line of equation (40) vanish. As a consequence the orthogonality constraints are fulfilled for these states. The eigenvalues obtained for the Hartree-Fock-Bogoliubov groundstate are the extremal ones. For correlated states these eigenvalues can only be reduced. More precisely, the range of the set of possible eigenvalues $L^{(1)}$, ... $L^{(4)}$ lies in the convex volume bounded by the extremes given above. For an interaction quadratic in the operators L the energy assumes extremal eigenvalues for extremal eigenvalues L in the case of symmetry breaking. Without symmetry breaking the eigenvalues would vanish. We have argued before in favour of only one non-vanishing eigenvalue $L^{(i)}$. Reduced to SO(5) this would be λ_1, whereas the second largest (vanishing one) is λ_2 of the representation (λ_1, λ_2). These correspond to the representations $(\lambda_1,0)$ actually found in the numerical calculations [4,3].

5 Conclusion

We have shown that the orthogonality constraints introduced by Zhang in his SO(5)-theory of high T_c-superconductivity play an important role in the mechanism for the transition from antiferromagnetism to superconductivity as a function of doping. We have further shown that these constraints are not strictly fulfilled, but that their fulfillment yields a maximum of the entropy (for fixed $\sum L_{a,b}^2$). At low temperatures the entropy plays a weaker role. However, if the interaction drives the groundstate to the case of extremal eigenvalues $L^{(i)}$, which may be very well the case for an interaction bilinear in the operators L, then again the orthogonality constraints are fulfilled.

We have expanded our scheme to a (mathematically natural) SO(8)-scheme. In this scheme two types of solutions for maximal entropy or extremal eigenvalues appear. Since the added degrees of freedom are probably massive, only those solutions, for which one eigenvalue is different from zero and the other ones vanish yield the minimum in the free energy.

These considerations did not take the microscopic interaction seriously into account. Work in this direction has to be done.

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Appendix A: Operators in an SO(8) space

A.1 Bilinear operators

All the operators in the SO(5) theory are of the form

$$N^+_{q,f,\gamma} = \frac{1}{2}\sum_{k,s,t} f(k) c^\dagger_{k+q,s} (\gamma\sigma^y)_{s,t} c^\dagger_{-k,t}, \tag{A.1}$$

$$N^0_{q,f,\gamma} = \frac{1}{2}\sum_{k,s,t} f(k) \gamma_{s,t} (c^\dagger_{k+q,s} c_{k,t} - \frac{1}{2}\delta_{q,0}\delta_{s,t}), \tag{A.2}$$

$$N^-_{q,f,\gamma} = \frac{1}{2}\sum_{k,s,t} f(k) c_{k+q,s} (\sigma^y\gamma)_{s,t} c_{-k,t}. \tag{A.3}$$

Here the summation k runs over the Brillouin zone. The vector q can either be 0 or q_0, where $2q_0$ is a reciprocal lattice vector. The staggered magnetization is described by the wave-vector q_0 as above. The function $f(k)$ stands either for 1 or $g(k)$ with $g(k) = g(-k) = -g(k+q_0) = \pm 1$. Finally γ is a hermitean two by two matrix. It may be either the unit matrix or one of the Pauli matrices.

First we consider the symmetry of N^+. If we exchange the two $c^\dagger$-operators, then we obtain

$$N^+_{q,f,\gamma} = N^+_{q,f(.+q),\sigma^y\gamma^T\sigma^y}. \tag{A.4}$$

One has

$$f(.+q) = s_{q,f} f \quad \text{with} \quad s_{q,f} = \begin{cases} 1 \text{ for } q = 0 \text{ or } f = 1, \\ -1 \text{ for } q = q_0 \text{ and } f = g \end{cases} \tag{A.5}$$

and

$$\sigma^y\gamma^T\sigma^y = s_\gamma\gamma \quad \text{with} \quad s_\gamma = \begin{cases} +1 \text{ for } \gamma = 1 \\ -1 \text{ for Pauli matrices} \end{cases}. \tag{A.6}$$

From this we conclude that only the six operators $N^+_{0,1,1}$, $N^+_{0,g,1}$, $N^+_{q_0,1,1}$, $N^+_{q_0,g,\sigma_\alpha}$ with $s_{q,f}s_\gamma = 1$ are different from zero. The same holds for N^-.

The hermitean adjoint operators are

$$(N^-_{q,f,\gamma})^\dagger = s_{q,f} N^+_{q,f,\gamma^\dagger}, \tag{A.7}$$

$$(N^0_{q,f,\gamma})^\dagger = s_{q,f} N^0_{q,f,\gamma^\dagger}. \tag{A.8}$$

We obtain for the commutators

$$[N^+_{q,f,\gamma}, N^+_{q',f',\gamma'}] = 0, \tag{A.9}$$

$$[N^-_{q,f,\gamma}, N^-_{q',f',\gamma'}] = 0, \tag{A.10}$$

$$[N^-_{q,f,\gamma}, N^+_{q',f',\gamma'}] = -2N^0_{q'-q,ff'(.-q),\gamma\gamma'}, \tag{A.11}$$

$$[N^-_{q,f,\gamma}, N^0_{q',f',\gamma'}] = N^-_{q-q',f(.-q')f',\gamma\gamma'}, \tag{A.12}$$

$$[N^0_{q,f,\gamma}, N^+_{q',f',\gamma'}] = N^+_{q+q',f(.+q')f',\gamma\gamma'}, \tag{A.13}$$

$$[N^0_{q,f,\gamma}, N^0_{q',f',\gamma'}] = \frac{1}{2}(N^0_{q+q',f(.+q')f',\gamma\gamma'} - N^0_{q+q',ff'(.+q),\gamma'\gamma}). \tag{A.14}$$

A.2 Zhang's Operators

The operators introduced by Zhang, which obey the commutator relations (2) of an SO-group were

$$L_{5,1} = Q = N^0_{0,1,1}, \tag{A.15}$$

$$L_{1+\alpha,1} = \frac{1}{2}(\pi^\dagger_\alpha + \pi_\alpha), \pi^\dagger_\alpha = N^+_{q_0,g,\sigma^\alpha}, \tag{A.16}$$

$$L_{5,1+\alpha} = \frac{-\mathrm{i}}{2}(\pi^\dagger_\alpha - \pi_\alpha), \pi_\alpha = -N^-_{q_0,g,\sigma^\alpha}, \tag{A.17}$$

$$L_{1+\alpha,1+\beta} = \epsilon_{\alpha,\beta,\gamma} S_{0,\gamma}, S_{0,\gamma} = N^0_{0,1,\sigma^\gamma}, \tag{A.18}$$

$$n_1 = L_{1,0} = \frac{1}{2}(\Delta^\dagger + \Delta), \Delta^\dagger = \mathrm{i}N^+_{0,g,1}, \tag{A.19}$$

$$n_5 = L_{5,0} = \frac{\mathrm{i}}{2}(\Delta^\dagger - \Delta), \Delta = -\mathrm{i}N^-_{0,g,1}, \tag{A.20}$$

$$n_{1+\alpha} = L_{1+\alpha,0} = S_{q_0,\alpha} = N^0_{q_0,1,\sigma^\alpha}. \tag{A.21}$$

Here we have added $n_a = L_{a,0}$ to the group, since they obey the same commutator relations.

A.3 Extension to operators obeying an SO(8) group

Obviously one can expand the range of operators $L_{a,b}$ by including the other operators N introduced above so that any pairs of particles, of holes or particle-hole pairs with total momentum 0 or q_0 in the singlet and triplet channel appear. This allows us to introduce components $L_{a,b}$ with $a, b = 6$ or 7. This expansion does not imply, that the symmetry group for the phase transition will be enlarged. Actually one expects that the new components of the "order-parameter" stay massive at the transition and will not contribute directly to the symmetry-breaking.

It is well-known [11,12] that there are additional operators adding or removing two electrons, $\eta^\dagger$ and η, which commute with the Hubbard Hamiltonian, which allows us by means of the commutator relations (2) to introduce

$$L_{1,6} = \frac{\mathrm{i}}{2}(\eta - \eta^\dagger), \eta^\dagger = N^+_{q_0,1,1}, \tag{A.22}$$

$$L_{5,6} = \frac{1}{2}(\eta^\dagger + \eta), \eta = N^-_{q_0,1,1}, \tag{A.23}$$

$$L_{1+\alpha,6} = -N^0_{0,g,\sigma^\alpha}, \tag{A.24}$$

$$n_6 = L_{6,0} = \mathrm{i}N^0_{q_0,g,1}. \tag{A.25}$$

Finally there are 7 more operators left, which fulfill the appropriate commutator relations with

$$L_{1,7} = \frac{1}{2}(\tilde\eta^\dagger + \tilde\eta), \tilde\eta^\dagger = N^+_{0,1,1}, \tag{A.26}$$

$$L_{5,7} = \frac{\mathrm{i}}{2}(\tilde\eta^\dagger - \tilde\eta), \tilde\eta = N^-_{0,1,1}, \tag{A.27}$$

$$L_{1+\alpha,7} = \mathrm{i}N^0_{q_0,g,\sigma^\alpha}, \tag{A.28}$$

$$L_{6,7} = -N^0_{q_0,1,1}, \tag{A.29}$$

$$n_7 = L_{7,0} = -N^0_{0,g,1}. \tag{A.30}$$

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