

Critical properties of projected SO(5) models at finite temperatures

E. Arrigoni and W. Hanke

Institut für Theoretische Physik, Universität Würzburg, D-97074 Würzburg, Germany

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We consider the projected SO(5) bosonic model introduced in order to connect the SO(5) theory of high- T_c superconductivity with the physics of the Mott-insulating gap, and derive the corresponding effective functional describing low-energy degrees of freedom. At the antiferromagnetic-superconducting transition, SO(5) symmetry-breaking effects due to the gap are purely quantum mechanical and become irrelevant in the neighborhood of a possible finite-temperature multicritical point separating the normal from the antiferromagnetic and the superconducting phases. A difference in the magnon and hole-pair mobility always takes the system away from the SO(5)-symmetric fixed point towards a region of instability, and the phase transition between the normal and the two ordered phases becomes first order before merging into the antiferromagnetic-superconducting line. Quantum fluctuations at intermediate temperatures, while introducing symmetry-breaking terms in the case of equal mobilities, tend to cancel the symmetry-breaking effects in the case of different mobilities.

I. INTRODUCTION

The SO(5) theory of high- T_c superconductivity¹⁻⁴ has been introduced as a concept to unify antiferromagnetism (AF) and d -wave superconductivity (SC) under a common symmetry principle. In order to study the physical consequences, and to make predictions to compare with experiments, several exact SO(5)-symmetric models with small symmetry-breaking terms have been proposed and investigated in detail.⁵⁻⁷ However, a shortcoming of these models, and of an *exact* SO(5) theory in general is that they are inconsistent with the antiferromagnetic gap at half filling, one of the most important features of the high- T_c cuprates.^{8,9} This can be understood by the fact that an SO(5) transformation “rotates” spin into charge and thus a requirement for an exactly SO(5)-invariant system would be to have the same charge and spin gap. This is in contradiction with the experimental situation in the high- T_c materials, where a large charge gap of some eV is present in the AF state at half filling, while spin-wave excitations are ungapped. The introduction of a *small* symmetry-breaking term,^{1,5,6,10,11} while on the one hand correctly selecting the AF state at half filling and shifting the AF-SC transition to finite doping, does not introduce a charge gap of the correct order of magnitude. In contrast, in a weakly coupled Hubbard ladder model, a spin and a charge gap of the same size are present and, in fact, it has been shown that SO(5) symmetry is dynamically restored at half filling.^{12,13}

In order to cure this problem at strong coupling as well, a class of SO(5) models—“projected” SO(5) models—has been introduced where the Mott-Hubbard gap is taken into account by means of a Gutzwiller projection, whereby doubly occupied states are projected out.¹⁴ In that paper, it was shown that, despite the symmetry-breaking effects of the projection, static correlation functions remain exactly SO(5) symmetric within a mean-field approximation. This is due to the fact that, neglecting dynamic effects, the Hamiltonian is manifestly SO(5) invariant. However, dynamic effects breaking the SO(5) symmetry become important whenever quan-

tum fluctuations are taken into account.¹⁴ In another paper,^{15,16} it was shown that the projection is crucial in order to correctly relate the d -wave superconducting gap at finite doping with the d -wave modulation of the AF gap observed at half filling by ARPES experiments.¹⁷

In a microscopic physical system, one would in general expect SO(5) symmetry to be explicitly broken by several terms. This is certainly the case for the Hubbard model, for example. However, it often occurs in nature that a symmetry, which is broken on the microscopic level, is then restored in the long-wavelength limit. Concerning SO(5), this has been shown to happen for quite generic ladder systems of the Hubbard type.^{12,13} Recently, Murakami and Nagaosa argued that the bicritical point of the AF to SC transition in the organic superconductor κ -(BEDT-TTF)₂X [Bis(ethylenedithio)tetrathiafulvalene] with $X = \text{Cu}[\text{N}(\text{CN})_2]\text{Cl}$, shows SO(5) critical exponents.¹⁸ In fact, one of the scenarios suggested by Zhang¹ is that there might be a direct first-order AF-to-SC transition terminating at a finite-temperature bicritical point, where the SO(5) symmetry is asymptotically restored at long wavelengths.¹ These ideas are very interesting from an experimental point of view, and open the possibility of an explicit test of SO(5) symmetry, via a direct “measurement of the number 5.”¹⁹ This could be done, as suggested in Ref. 18, by measuring the critical exponents of the AF-to-SC transition, which, given the spatial dimensionality, should only depend on the number of components n of the order parameter. On the other hand, it is well known that for $n > n_c \approx 4$, the SO(5) symmetric fixed point is unstable towards a so-called biconical fixed point.²⁰ However, since $n = 5$ is close to n_c , it turns out that the stable biconical fixed point only breaks the symmetry by about 20%.

However, the situation of the high- T_c materials is quite delicate. As discussed above, the Mott-Hubbard gap plays an important role, and it produces a *substantial* breaking of the SO(5) symmetry. In Ref. 14, it was shown that in the extreme case of a Gutzwiller projection, a degree of freedom is eliminated completely and the real and imaginary part of the local superconducting parameter become conjugate variables. Therefore it is not clear whether such a *projected* SO(5) symmetry can become asymptotically a *complete*

SO(5) symmetry in the neighborhood of some critical point.

In this paper, we show why symmetry-breaking effects due to the projection are asymptotically irrelevant in the neighborhood of a finite-temperature critical point. However, two kinds of symmetry-breaking effects tend to prevent SO(5) symmetry from being restored asymptotically. One is related with the different mobilities of hole pairs and magnons ($\eta \neq 1$ below), and the second one is due to the renormalization effects from quantum fluctuation at an intermediate length scale. The common tendency of these effects is to draw the system into a region of instability, where the two AF/normal (N) and SC/ N transitions become first order before merging at the AF/SC/ N triple point.^{20,18} However, when the first effect is large, quantum fluctuations tend to take the system back to the SO(5) point.

This paper is organized as follows: In Sec. II we start from the projected SO(5)-symmetric model (allowing for a symmetry-breaking term η in the mobilities), and treat it by a slave-boson functional-integral approach in order to deal with the hard-core constraint. The important result is that at the AF-SC transition, the *classical* part of the action of the *projected* model preserves its SO(5) structure at $\eta=1$, despite the symmetry-breaking terms arising from the projection. These terms only appear in the *quantum-mechanical* (i.e., time derivative) part of the action. This fact gives a rigorous justification for the much used semiclassical description of the high- T_c materials via a SO(5)-symmetric model^{21,10,11} despite of the presence of the large Hubbard gap. In Sec. III, we derive the associate effective Ginzburg-Landau model by integrating out the momenta conjugate to the AF superspin variables.²² We study the properties of such model in the neighborhood of the AF/SC/ N triple point and discuss the possibility of SO(5) symmetry restoring at long wavelengths.

In Sec. IV, we evaluate the corrections to the effective classical action due to the so far neglected quantum fluctuations. For small temperatures, these mainly affect the magnon-magnon scattering, thus breaking the SO(5) symmetry. Finally, in Sec. V we draw our conclusions. Some details of the calculations are given in the appendixes.

II. MODEL

We start from the effective bosonic model introduced in Refs. 23 and 14, which describes low-energy *bosonic* excitations of ‘‘blocks,’’ (also referred to as ‘‘sites’’) labeled by the coordinate x , consisting of a rung in a one-dimensional (1D) ladder or of a 2×2 plaquette in a 2D system.

$$H = \bar{\Delta}_s \sum_x t_a^\dagger(x) t_\alpha(x) + \bar{\Delta}_c \sum_x t_i^\dagger(x) t_i(x) - \bar{J}_s \sum_{\langle xx' \rangle} n_\alpha(x) n_\alpha(x') - \bar{J}_c \sum_{\langle xx' \rangle} n_i(x) n_i(x'). \quad (1)$$

In this paper, we shall use similar conventions as in Ref. 14, where the indices a, b, \dots are the SO(5) superspin indices and take the values 1,2,3,4,5 (in some cases, they might also include the ‘‘hole’’ index h), $\alpha, \beta, \dots = 2,3,4$ (corresponding to x, y, z) denote the spin indices and $i, j = 1,5$ denote the charge indices, and repeated indices are implicitly summed

over. A boldface sign indicates the vector as a whole. Here, $\bar{\Delta}_s$ is the energy required to produce a magnon excitation, i.e., to replace a singlet with a triplet in a block, while $\bar{\Delta}_c$ is the energy required in order to produce a particle or hole pair. It is clear that $\bar{\Delta}_c$ is of the order of the Mott-Hubbard gap and thus $\bar{\Delta}_c \gg \bar{\Delta}_s$. On the other hand, \bar{J}_s and \bar{J}_c describe the hybridization of these excitations between nearest-neighbor sites and are related to their mobility. The Hamiltonian Eq. (1) acts on a ‘‘vacuum’’ $|\Omega\rangle$, which is a kind of ‘‘RVB’’ state consisting of a product state of half filled singlet states $|\Omega(x)\rangle$ in each block. On the other hand, the fivefold states $t_a^\dagger(x)|\Omega(x)\rangle$ describe the triplet magnon states (for $a=2,3,4$), and the d -wave hole and particle pair states on a block ($a=1,5$).²³ More specifically, one can define the charge eigenoperators t_h and t_p as

$$t_1 = \frac{1}{\sqrt{2}}(t_h + t_p) \quad t_5 = \frac{1}{i\sqrt{2}}(t_h - t_p), \quad (2)$$

where t_h^\dagger is the creation operator for a hole pair and t_p^\dagger is the creation operator for a particle pair. In Eq. (1), the n_a play the role of ‘‘displacement’’ coordinates of local harmonic oscillators, while we will denote with p_a the conjugate momenta, and we have the transformation to canonical variables:

$$t_a = \frac{1}{\sqrt{2}}(n_a + ip_a). \quad (3)$$

Due to their microscopic origin these bosonic states are hard-core bosons, in the sense that at most one boson can reside on each site. Mathematically, this is expressed by the condition

$$\sum_a t_a^\dagger(x) t_a(x) \leq 1. \quad (4)$$

The particle and hole density is controlled by the chemical potential μ , which couples to the Hamiltonian via a term

$$H_\mu = -2\mu \sum_x [t_p^\dagger(x) t_p(x) - t_h^\dagger(x) t_h(x)]. \quad (5)$$

In the presence of this chemical potential term, the gap energy of the hole and particle pairs become $\bar{\Delta}_c + 2\mu$ and $\bar{\Delta}_c - 2\mu$, respectively. A (negative) chemical potential of the order of the charge gap $\bar{\Delta}_c/2$ is needed to induce an AF-SC transition in this system. Near such a transition point, the gap energy of the hole pair $\bar{\Delta}_c + 2\mu$ can be comparable to the (local) spin gap $\bar{\Delta}_s$, while the gap towards a particle pair excitation is pushed up and becomes of the order of twice the charge gap. Since this is a very large energy scale, we can safely project this excitation out of the spectrum in the low-energy limit, by requiring that the condition

$$t_p(x)|\Psi\rangle = 0 \quad (6)$$

is fulfilled at every site x . The new Hamiltonian takes the form

$$\begin{aligned}
H = & \bar{\Delta}_s \sum_{x,\alpha} t_a^\dagger(x) t_\alpha(x) + (\bar{\Delta}_c + 2\mu) \\
& \times \sum_x t_h^\dagger(x) t_h(x) - \bar{J}_s \sum_{\langle x,x' \rangle, \alpha} n_\alpha(x) n_\alpha(x') \\
& - \bar{J}_c/2 \sum_{\langle x,x' \rangle} [t_h^\dagger(x) t_h(x') + \text{H.c.}]. \quad (7)
\end{aligned}$$

In Ref. 14 it was shown that the constraint Eq. (6) can be enforced by introducing canonical commutation rules between the two variables n_1 and n_5 , i.e.,

$$[n_1, n_5] = i/2, \quad (8)$$

and therefore we can identify $\sqrt{2}n_1$ with the ‘‘hole displacement’’ n_h and $\sqrt{2}n_5$ with its conjugate momentum p_h . The SO(5) structure of the Hamiltonian becomes now clear if one introduces the superspin vector

$$m_a \equiv (\eta n_h, n_2, n_3, n_4, \eta p_h), \quad (9)$$

where, for convenience, we have absorbed the different mobility for hole pairs and magnons $\eta \equiv \sqrt{\bar{J}_c/2\bar{J}_s}$ into the definition of the superspin. Carrying out the transformation to canonical variables Eq. (3), the Hamiltonian Eq. (7) now takes the simple form

$$\begin{aligned}
H = & \frac{\Delta_s}{2} \sum_x p_\alpha(x)^2 + \frac{\Delta_s}{2} \sum_x m_\alpha(x)^2 + \frac{\Delta_c}{2} \sum_x m_i(x)^2 \\
& - J \sum_{\langle xx' \rangle} m_a(x) m_a(x'), \quad (10)
\end{aligned}$$

where we have further redefined

$$\Delta_c \equiv \frac{\bar{\Delta}_c + 2\mu}{\eta^2}, \quad \Delta_s \equiv \bar{\Delta}_s, \quad \text{and } J \equiv \bar{J}_s. \quad (11)$$

The anisotropy in superspin space due to η reflects now into the constraint, as we will see in Eq. (16) below. If one forgets for a moment the connection between coordinates m_a and their conjugate momenta, the Hamiltonian Eq. (10) becomes exactly SO(5) invariant under rotation of the superspin Eq. (9) at the AF-SC transition point $\Delta_s = \Delta_c$, which is reached by changing the chemical potential μ , i.e., at the AF-SC transition. If one further has $\eta = 1$, i.e., $2\bar{J}_s = \bar{J}_c$, the constraint is invariant as well, and one apparently has a complete SO(5) symmetric model (cf. Ref. 14). More specifically, one would like to SO(5) ‘‘rotate’’ just the m_a coordinates, leaving the conjugate coordinates to the magnon part p_α unrotated. This is possible, for example, in a classical ensemble, where, due to Liouville’s theorem, expectation values are evaluated with the measure $\prod_i dp_i dq_i \times \exp[-H[p_i, q_i]]$, and rotations of the q_i only leaves it invariant. Of course, this does not hold for dynamics, which is affected by the relation between the two ‘‘superconducting’’ canonically conjugate components m_1/η and m_5/η , and between the AF components m_α and their conjugate momenta p_α . Thus SO(5) symmetry is broken in dynamics, as pointed out in Ref. 14. Unfortunately, the relation between conjugate variables is also important in quantum-mechanical *static* av-

erages, so that ground-state or finite-temperature averages are generally expected to break the symmetry when the full quantum problem is taken into account.

In order to understand the nature of the symmetry-breaking terms, it is convenient to go over to a functional-integral representation of the partition function for the Hamiltonian Eq. (7). The hard-core constraints can be conveniently taken care of by means of a slave-boson representation,²⁴ where the boson operator $e(x)$ labeling ‘‘empty’’ sites is introduced. The detailed procedure is shown in Appendix A. After this transformation, the action takes the form

$$S = S_{QM} + S_{CL}, \quad (12)$$

where

$$\begin{aligned}
S_{QM} = & \int_0^\beta d\tau \sum_x \left[-ip_\alpha(x, \tau) \dot{m}_\alpha(x, \tau) \right. \\
& \left. - \frac{i}{\eta^2} m_5(x, \tau) \dot{m}_1(x, \tau) \right] \quad (13)
\end{aligned}$$

(\dot{m}_a indicates the time derivative of m_a), has the well-known form $p\dot{q}$ of the Feynman path integral, the i coming from the imaginary-time representation. Moreover,

$$\begin{aligned}
S_{CL} = & \int_0^\beta d\tau \left(\frac{\Delta_s}{2} \sum_x p_\alpha(x, \tau)^2 + \frac{\Delta_s}{2} \sum_x m_\alpha(x, \tau)^2 \right. \\
& + \frac{\Delta_c}{2} \sum_x m_i(x, \tau)^2 - J \sum_{\langle xx' \rangle} e(x, \tau) m_a(x, \tau) \\
& \left. \times e(x', \tau) m_a(x', \tau) \right), \quad (14)
\end{aligned}$$

where we have to replace

$$e(x, \tau) = \sqrt{1 - \frac{p_\alpha(x, \tau)^2}{2} - \frac{m_\alpha(x, \tau)^2}{2} - \frac{m_i(x, \tau)^2}{2\eta^2}}, \quad (15)$$

which implicitly includes the condition

$$\frac{p_\alpha(x, \tau)^2}{2} + \frac{m_\alpha(x, \tau)^2}{2} + \frac{m_i(x, \tau)^2}{2\eta^2} \leq 1, \quad (16)$$

and where we have already carried out the transformation to canonical coordinates, Eq. (3), for the corresponding fields.²⁵ Equation (14) is the correct classical limit of a *projected*, i.e., of the *physical* SO(5) model. Notice that the effects of the hard-core constraint is to introduce a renormalization of the boson hopping, and to bound the superspin magnitude, without, however, fixing its length.²⁶ Thus the requirement that the superspin magnitude be unity should not be taken as a rigorous constraint of the SO(5) theory, at least not of the

projected one (which is the physical one). On the other hand, one expects that in the homogeneous ordered phase this constraint might be a good assumption. A similar result has been shown by Wegner,²⁷ namely, that the orthogonality constraint in the exact SO(5) model is not a rigorous constraint, but it is favored at high temperature, as it maximizes the entropy.

Equation (12) clearly identifies the SO(5)-symmetry breaking terms. The classical action S_{CL} is *exactly* SO(5) invariant at the AF-SC transition ($\Delta_s = \Delta_c$) and for $\eta = 1$, while apparently incurable symmetry-breaking terms come from the time-derivative terms in S_{QM} . More specifically, with these values of the parameters, if one carries out an SO(5) rotation within the superspin vector, Eq. (9), S_{CL} remains invariant, while S_{QM} is changed. If quantum fluctuations are neglected, one can choose time-independent fields and set Eq. (13) to zero. In this case, any equilibrium expectation value is exactly SO(5) invariant. More specifically, let us take a generic SO(5) rotation matrix $R(\mathbf{n}) = \exp i n_a \Gamma_a$ parametrized by the vector \mathbf{n} [Γ_a are the SO(5) generators⁵], and $f[\mathbf{m}(x), \mathbf{p}(x)]$ is a function of the superspin vector $\mathbf{m}(x)$, and, possibly, of $\mathbf{p}(x)$. Then, the classical expectation values $\langle \dots \rangle_{CL}$ have the property

$$\langle f[\mathbf{m}(x), \mathbf{p}(x)] \rangle_{CL} = \langle f[\mathbf{R} \cdot \mathbf{m}(x), \mathbf{p}(x)] \rangle_{CL}, \quad (17)$$

which is the requirement of SO(5) invariance. Notice that the p_α should not be rotated, while in an exact SO(5) model they should.

The question is: when is it justified to neglect the time dependence of the fields? This is allowed at moderately high temperatures, more precisely, at temperatures much larger than v/ξ (in units of $k_B = \hbar = 1$), where ξ is the correlation length and v is a typical velocity, in our case equal to Ja , a being the lattice spacing. This means that neglecting S_{QM} is *exactly justified* when ξ becomes infinite, i.e., in the neighborhood of a finite-temperature critical point, as a possible (finite temperature) multicritical point at which the AF/N and the SC/N transition lines merge into a first-order line.¹ Moreover, this critical point is indeed a good candidate for a possible asymptotic restoring of the *complete* SO(5) symmetry even in the presence, microscopically, of a *projected* SO(5) symmetry. This is very important as it would mean that the large-energy symmetry-breaking effect of the Mott-insulator gap would be exactly compensated at this critical point. This is analogous to the well-known situation for the antiferromagnetic spin-flop transition^{1,28,29,30} where a system with uniaxial anisotropy restores SO(3) symmetry at the bicritical point. However, there are some important differences with respect to the spin-flop transition, as we will show in the next sections. Moreover, notice that due to the symmetry breaking term, Eq. (13), it is unlikely that SO(5) symmetry can be restored if the AF-SC transition is controlled by a quantum-critical point. Since we are interested in finite-temperature critical points, we will restrict to the case of three spatial dimensions D .

III. EFFECTIVE GINZBURG-LANDAU ACTION

In this section, we study the action Eq. (10) in more detail. We first integrate out the momenta p_α and obtain an effective action restricted to the superspin variables. For tem-

peratures smaller than the singlet-triplet splitting Δ_s , one can restrict to a Gaussian integration of the momenta, i.e., consider only quadratic terms in p_α . Carrying out such an expansion, one obtains

$$S_{CL} = S_{pm} + S_m + \mathcal{O}(p_\alpha^4), \quad (18)$$

where, leaving the τ dependence implicit

$$S_m = \int_0^\tau d\tau \left(\frac{\Delta_s}{2} \sum_x m_\alpha(x)^2 + \frac{\Delta_c}{2} \sum_x m_i(x)^2 - J \sum_{\langle xx' \rangle} r(x) m_\alpha(x) r(x') m_\alpha(x') \right), \quad (19)$$

$$S_{pm} = \int_0^\tau d\tau \sum_x \frac{\Delta_s}{2} \mathcal{A}(x) p_\beta(x)^2, \quad (20)$$

where we have defined

$$\mathcal{A}(x) \equiv 1 + \frac{2J}{\Delta_s} \frac{m_\alpha(x)}{4r(x)} \sum_d^{nn} m_\alpha(x+d) r(x+d), \quad (21)$$

$$r(x) \equiv \sqrt{1 - \frac{m_\alpha(x)^2}{2} - \frac{m_i(x)^2}{2\eta^2}}, \quad (22)$$

and the sum \sum_d^{nn} extends over nearest-neighbor sites.

It is now convenient to reabsorb the \mathbf{m} -dependent coefficient $\mathcal{A}(x)$ of the \mathbf{p}^2 term into the definition of the momenta \mathbf{p} . This is done in order to avoid the appearance of terms depending on the amplitude of the imaginary-time slice in the effective action. Furthermore, in order to avoid a \mathbf{m} -dependent Jacobian due to the transformation, it is convenient to transform the \mathbf{m} coordinates in such a way that the Jacobian remains unity. The general procedure is illustrated in Appendix B. Up to second order in \mathbf{m}^2 , the new \mathbf{m}' coordinates are related with the old ones via

$$m_\alpha(x) = m'_\alpha(x) \left(1 + \frac{3J}{7\Delta_s} |\mathbf{m}'(x)|^2 \right). \quad (23)$$

After this transformation, the integration of the $p'_\alpha(x) \equiv p_\alpha(x) \sqrt{\mathcal{A}(x)}$ only affects S_{QM} , and one obtains a new QM action in the form

$$S'_{QM} = \int_0^\beta d\tau \int dx \left(\frac{\dot{m}_\alpha^2}{2\Delta_s \mathcal{A}(x)} - \frac{i}{\eta^2} m_5(x) \dot{m}_1(x) \right), \quad (24)$$

where the transformation Eq. (23) should be inserted, and we have absorbed the unit cell volume $\mathcal{V} = a^3$ in the definition of the fields by renaming $m_a^2/\mathcal{V} \rightarrow m_a^2$.

Thus the total effective SO(5) action restricted to the superspin variables is given by Eq. (19) plus Eq. (24). The transformation Eq. (23) must still be carried out on the m variables, but, due to the fact that the coefficient $3J/7\Delta_s$ is small at the transition, this does not change the result significantly. On the other hand, it is important to take into account the effects of the hard-core constraint, which introduces the transformation Eq. (22), and, implicitly, the restriction of the superspin within a five-dimensional hypersphere (or a ellip-

soid, if $\eta \neq 1$).²⁶ Thus S_m [Eq. (19)] gives an effective classical functional microscopically derived from an SO(5) model,²² where the physics of the Mott insulating gap has been properly taken into account via the projection. This is the appropriate functional which should be used for *physical* predictions of the SO(5) theory, consistent with the gap.

Close to the phase transitions, it is more convenient to derive a Ginzburg-Landau form for the action, obtained, as usual, by expanding in powers of the field \mathbf{m} and keeping only lowest-order gradient terms. After inserting Eq. (23) and dropping the prime indices in the fields \mathbf{m} , we obtain

$$S'_{CL} = \int_0^\beta d\tau \int dx \left[\frac{r_s}{2} m_\alpha(x)^2 + \frac{r_c}{2} m_i(x)^2 + \frac{\rho}{2} [\vec{\nabla} m_\alpha(x)]^2 + \frac{u_s}{8} \left(\sum_\alpha m_\alpha(x)^2 \right)^2 + \frac{u_c}{8} \left(\sum_i m_i(x)^2 \right)^2 + \frac{u_{cs}}{4} \left(\sum_\alpha m_\alpha(x)^2 \right) \left(\sum_i m_i(x)^2 \right) \right], \quad (25)$$

with the parameters

$$\begin{aligned} \frac{r_{s/c}}{2} &= \left(\frac{\Delta_{s/c}}{2} - DJ \right), \\ \frac{\rho}{2} &= \frac{Ja^2}{2}, \\ \frac{u_s}{8} &= \frac{\mathcal{V}J}{2} \left(D + \frac{3r_s}{7\Delta_s} \right), \\ \frac{u_c}{8} &= \frac{\mathcal{V}J}{2} \left(\frac{D}{\eta^2} + \frac{3r_c}{7\Delta_s} \right), \\ u_{cs} &= \frac{u_c + u_s}{2}, \end{aligned} \quad (26)$$

where we have considered the fact that³⁹

$$\begin{aligned} \mathcal{V} \sum_x m(x) \sum_d^{nn} m(x+d) &= \frac{\mathcal{V}}{2} \sum_x \sum_d^{nn} \{ m(x)^2 + m(x+d)^2 - [m(x) - m(x+d)]^2 \} \\ &\approx 2D \int dx m(x)^2 - a^2 \int dx [\vec{\nabla} m(x)]^2. \end{aligned} \quad (27)$$

The critical properties of the model Eq. (25) have been analyzed in several works.^{20,28,30,31,29,32,18} Its phase diagram is determined by two relevant parameters, the first one $r_s - r_c \propto \Delta_s - \Delta_c$ controls the transition between the AF and the SC phases, while the other $\sim \min(r_s, r_c)$ controls the second-order transition between the appropriate ordered (AF or SC) and the disordered phase. At the transition point $r_s \sim r_c \sim 0$, there are two competing fixed points controlling the transition,²⁰ the Heisenberg bicritical fixed point [in this specific case, the SO(5) fixed point], and the biconical tetracritical fixed point. According to the ϵ expansion, the latter fixed

point turns out to be the stable one for $n > n_c \approx 4 - O(\epsilon)$. This means that, in general, the model Eq. (25), which has $n=5$, is expected to flow to this latter fixed point and not to the SO(5)-symmetric one for $u_s \neq u_c \neq u_{cs}$. On the other hand, since $n=5$ is not very far away from n_c , the stable biconical fixed point is approximately SO(5) invariant with symmetry-breaking terms of the order of 20%. Moreover, there is a plane in the u_s, u_c, u_{cs} space, given by the condition $u_{cs}^2 = u_c u_s$, from which the system flows to the SO(5) point.^{20,18} This is due to the fact that a scale transformation of, say, the SC components $m_i^2 \rightarrow m_i^2 u_s / u_c$ of the order parameter would yield again an SO(5)-symmetric interaction of the form $u |\mathbf{m}|^4$. The asymmetry would then be transferred into different susceptibilities ρ_s, ρ_c for the AF and for the SC order parameters. However, it has been shown in Refs. 33,29 that the different in the susceptibilities is an irrelevant parameter.

In our case, we have

$$\Delta u^2 \equiv u_{cs}^2 - u_c u_s = \left(\frac{u_c - u_s}{2} \right)^2 \geq 0 \quad (28)$$

which means that the SO(5) symmetric fixed point is never reached, except when the equal sign holds, i.e., when $\eta \neq 1$ (at the transition $r_s = r_c$). On the other hand, we expect on physical grounds the mobility of the hole pairs to be smaller than that of the magnons, and thus η to be smaller than 1. Unfortunately, for the case Eq. (28), the couplings flow away into a region of instability. The common interpretation is that the AF/N and SC/N transitions become first order as well (fluctuation-induced first-order transition), at least close enough to the AF/SC/N triple point.^{20,18}

This fact seems in contrast with the apparent observation of bicritical behavior with SO(5) critical exponents in the organic superconductor κ -(BEDT-TTF)₂X (see Refs. 34 and 35), by Murakami and Nagaosa.^{18,36} There may be several ways to understand this. One possibility is that other effects not considered here, such as, e.g., Coulomb interactions, fermionic excitations,¹⁵ or quantum effects, as discussed in Sec. IV, counterbalance this effect and draw the system back to the domain of attraction of the biconical fixed point. As discussed above, the differences between the SO(5) and the biconical fixed point are only about 20%, so that they might be not observable experimentally. Alternatively, since the flow would cross the SO(5) plane, it could produce SO(5) exponents at intermediate length scales. On the other hand, Hu and co-workers^{37,38} observe a coexistence region of AF and SC for the SO(5)-anisotropic case, which could be possibly identified with the biconical phase. Their result could be due to the fact that they consider a different c -axis anisotropy (χ in Ref. 39), for the AF and for the SC variables.

IV. QUANTUM CORRECTIONS

Even when considering a classical (i.e., finite-temperature) critical point, the quantum-mechanical symmetry-breaking terms S_{QM} although irrelevant in the renormalization-group (RG) sense, contribute to the RG flow up to a certain length scale of the order of v/T . Since S_{QM} breaks the SO(5) symmetry, it is expected, during this initial renormalization process, to introduce symmetry-breaking

terms in S_{CL} . Therefore, even when S_{CL} is SO(5) symmetric at the microscopic scale, the renormalized S_{CL} at the scale $\xi \sim v/T$ will probably break the symmetry. In this section, we evaluate these symmetry-breaking terms originating from S_{QM} , or, more precisely, from the time dependence of the fields.

In order to evaluate these effects, we separate the fields into their static and dynamic parts, and integrate out the latter. Since we are working at finite temperature, we have to integrate out the components of the fields with Matsubara frequencies $\omega_n = 2\pi nT$ with $n \neq 0$. In order to obtain an analytic expression for these corrections, we restrict to one-loop contributions and take just the leading low-temperature terms.

We first diagonalize the noninteracting (quadratic) part of the action Eq. (24) plus Eq. (25) by Fourier transform. We can neglect the corrections to S'_{QM} due to the transformation to the primed variables Eq. (23), as it introduces irrelevant quartic time-derivative terms. In Fourier space, the action takes the usual form

$$\begin{aligned} S'_{QM} + S'_{CL} = & \frac{1}{2} \sum_k m_a(-k) [G(k)^{-1}]_{ab} m_b(k) \\ & + \frac{1}{8} \sum_{k_1, k_2, k_3} m_a(k_1) m_a(k_2) u_{ab} \\ & \times m_b(k_3) m_b(-k_1 - k_2 - k_3), \end{aligned} \quad (29)$$

where we have introduced the shorthand notation $k \equiv (k, \omega)$, and $\sum_k \equiv (1/\beta) \sum_{\omega} \int^{\Lambda} [d^3k / (2\pi)^3]$, with $\Lambda \sim 1/a$ a short-distance cutoff for k . In Eq. (29), the nonzero elements of the (noninteracting) Green's functions read

$$G(k)_{\alpha\beta} = \frac{\delta_{\alpha,\beta}}{r_s + \frac{\omega^2}{\Delta_s} + \rho k^2}, \quad (30)$$

$$G(k)_{1,1} = G(k)_{5,5} = \frac{\rho k^2 + r_c}{(\rho k^2 + r_c)^2 + \frac{\omega^2}{\eta^4}}, \quad (31)$$

and

$$G(k)_{5,1} = -G(k)_{1,5} = \frac{\frac{\omega}{\eta^2}}{(\rho k^2 + r_c)^2 + \frac{\omega^2}{\eta^4}}, \quad (32)$$

and the interaction parameters are $u_{\alpha,\beta} = u_s$, $u_{i,j} = u_c$, and $u_{i,\alpha} = u_{cs}$.

At one loop, integration of the $\omega \neq 0$ fields only changes the parameters r , and u , similarly to conventional field theory. In the $T \rightarrow 0$ limit, the change of the former is finite, and merely shifts the transition point. On the other hand, the changes δu_{ab} in the interaction parameters u_{ab} grow logarithmically with decreasing temperature at the critical point.

We will, thus, restrict to evaluation of these corrections. These are given by the sum of the usual ‘‘loop’’ diagrams, which give

$$\delta u_{ab} = -\frac{1}{2} \sum_c u_{ac} u_{cb} I_{cc} - 2u_{ab}^2 I_{ab} - u_{ab} (I_{aa} u_{aa} + I_{bb} u_{bb}), \quad (33)$$

where the integrals I_{ab} are given by

$$I_{ab} = \sum_{k, \omega \neq 0} G(k)_{aa} G(-k)_{bb}. \quad (34)$$

In Eqs. (33) and (34), we have neglected contributions from nondiagonal parts of Green's functions Eq. (32), as they only give finite contributions to integrals of the form Eq. (34) in the low-temperature limit. The same holds for integrals containing at least one Green's function of the superconducting fields Eq. (31). This is due to the fact that for these fields the (bare) dynamical critical exponent^{40,41} z is equal to 2, and it does not produce divergences in $D=3$. This in turn occurs because the two components of the SC order parameter are canonically conjugate, while the AF ones have independent massive ones. Therefore we will consider only the divergent contribution

$$I_{\alpha,\beta} = I_s \equiv \frac{1}{8\pi^2} \sqrt{\frac{\Delta_s}{\rho^3}} \ln \frac{\Lambda \sqrt{\rho \Delta_s}}{2\pi T}, \quad (35)$$

where we have assumed that we lie outside of the region of influence of the quantum critical fixed point, i.e., $T \gg \sqrt{r_{c/s} \Delta_s}$. Replacing Eq. (35) in Eq. (33), we obtain for the leading contributions

$$\begin{aligned} \delta u_s &= -\frac{11}{2} u_s^2 I_s, \\ \delta u_c &= -\frac{3}{2} u_c^2 I_s, \end{aligned} \quad (36)$$

$$\delta u_{cs} = -\frac{5}{2} u_s u_{cs} I_s.$$

As expected, quantum fluctuations draw the system away from the SO(5)-invariant point even in the case where $\eta = 1$. This can be seen by adding these corrections to an initially SO(5)-invariant system with $u_c = u_s = u_{cs} = u$. At the lowest order in the u_a , the renormalized parameters $u'_a = u_a + \delta u_a$ obey the relation

$$\Delta u'^2 \equiv u_{cs}'^2 - u_s' u_c' = 2I_s u^3 > 0, \quad (37)$$

i.e., as in the case of $\eta \neq 1$, Eq. (28), the system is drawn into the instability region where a fluctuation-induced first-order transition is expected. This indicates that quantum fluctuations and anisotropy $\eta \neq 1$ cooperate in the same direction and draw the system into the instability region, where no finite fixed point is expected. However, for the case where the u_a are different, one obtains

$$\Delta u'^2 - \Delta u^2 = -\frac{u_s}{2} (7u_{cs}^2 - 11u_c u_s) I_s. \quad (38)$$

Further inserting the values of the u_a from Eq. (26) with $\eta \neq 1$ (we fix ourselves at the triple point $r_s = r_c$), Eq. (38) becomes negative for $\eta < x_c$, or $\eta > 1/x_c$ with $x_c \approx 0.498$. Therefore, for large difference in the mobilities η , quantum fluctuations tend to shift the renormalized parameters back towards the domain of attraction of the biconical and of the SO(5) fixed point.

V. CONCLUSIONS

In conclusion, we have analyzed the properties of a projected SO(5) model which takes into account the high-energy physics of the Mott-insulating gap. As already pointed out in Ref. 14, the chemical potential can always be shifted to the AF-SC transition point in order to cancel the symmetry-breaking terms produced by the gap in the classical part of the action. On the other hand, symmetry-breaking terms due to the projection show up in the quantum-mechanical part of the action, as a conjugacy relation between the superconducting components of the superspin vector. A further source of symmetry breaking is due to the different mobility of the hole pairs and of the magnons parametrized by $\eta \neq 1$.

Close to the AF/SC/ N finite-temperature multicritical point, the quantum effects due to the projection are irrelevant, although subleading symmetry-breaking corrections appear at intermediate length scales. When considered separately, these symmetry-breaking effects both draw the RG flow into a region of instability with first-order transitions and no SO(5) symmetry. On the other hand, for strong anisotropies $\eta \lesssim 0.5$, quantum corrections partly cancel the symmetry-breaking effects.

There are possibly other effects, such as Coulomb interaction, or fermionic excitations, which can possibly take the system back into the domain of attraction of the biconical fixed point, where SO(5) symmetry is only broken by $\sim 20\%$. Notice that, since the order parameter must be rescaled in order to reach this fixed point, the (possibly approximate) SO(5) symmetry reached at this critical point is *renormalized*, in the sense of Ref. 12. This means, for example, that the SO(5) picture would be consistent with different absolute magnitudes of the SC and AF gaps, as observed experimentally.¹⁵

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APPENDIX A: EXACT SLAVE-BOSON TREATMENT OF THE CONSTRAINT

The hard-core constraint Eq. (4) becomes (after projecting out the electron pairs)

$$Q(x) = t_\alpha^\dagger(x)t_\alpha(x) + t_h^\dagger(x)t_h(x) + e^\dagger(x)e(x) - 1 = 0. \quad (\text{A1})$$

The ‘physical’ bosonic operators are then obtained as usual by the replacement

$$t_a(x) \rightarrow t_a(x)e^\dagger(x) \quad (\text{A2})$$

(including $a = h$), so that the constraint is now conserved by the Hamiltonian. Within the functional integral, the constraint Eq. (A1) can be enforced as usual by adding a ‘Lagrange multiplier’ term $i\sum_x \lambda(x)Q(x)$ and integrating over all $\lambda(x)$. The partition function can thus be written in terms of an integral over bosonic fields

$$\mathcal{Z} = \int \mathcal{D}t_\alpha^\dagger \mathcal{D}t_\alpha \mathcal{D}t_h^\dagger \mathcal{D}t_h \mathcal{D}e^\dagger \mathcal{D}e \mathcal{D}\lambda \exp - S', \quad (\text{A3})$$

with the action

$$\begin{aligned} S' = & \int_0^\beta d\tau \left\{ \sum_x \left[t_\alpha^\dagger(x, \tau) \left(\frac{\partial}{\partial \tau} + i\lambda(x) \right) t_\alpha(x, \tau) + t_h^\dagger(x, \tau) \right. \right. \\ & \times \left. \left(\frac{\partial}{\partial \tau} + i\lambda(x) \right) t_h(x, \tau) + e^\dagger(x, \tau) \left(\frac{\partial}{\partial \tau} + i\lambda(x) \right) \right. \\ & \left. \left. \times e(x, \tau) - i\lambda(x) \right] + H(\tau) \right\}, \quad (\text{A4}) \end{aligned}$$

where $H(\tau)$ is obtained by replacing Eq. (A2) in Eq. (7) and by replacing all bosonic operators with the corresponding fields at the imaginary time τ (since the Hamiltonian is already normal ordered). In principle, one should take a discretization of the time variable and consider the continuum limit only at the end of the calculation.^{42–44,25} Notice that the integration of λ would not give a constraint like Eq. (A1) for the bosonic fields at all imaginary times. Nevertheless, one can proceed in the usual way by carrying out the gauge transformation

$$\begin{aligned} e(x, \tau) &= \bar{e}(x, \tau) e^{i\theta(x, \tau)}, \\ t_a(x, \tau) &= \bar{t}_a(x, \tau) e^{i\theta(x, \tau)}, \\ \lambda(x) &= \bar{\lambda}(x, \tau) - \dot{\theta}(x, \tau), \end{aligned} \quad (\text{A5})$$

where $\bar{e}(x, \tau) = |e(x, \tau)|$. In this way, we can restrict to real values of the boson field e and absorb the time dependence of its phase into a (now) time dependent λ . Integration over $\lambda(x, \tau)$ now leads to the enforcement of the constraint via the δ function (for simplicity, we drop the bar everywhere)

$$\prod_{x, \tau} \delta[|t_\alpha(x, \tau)|^2 + |t_h(x, \tau)|^2 + e(x, \tau)^2 - 1] \quad (\text{A6})$$

at all imaginary times. Integration over $e(x, \tau)$ allows one to replace it everywhere in the Hamiltonian, leading to the new action Eq. (12) with Eq. (14).

APPENDIX B: INTEGRATION OF THE MOMENTA

The \mathbf{p} -dependent part of the action has the general form [cf. Eqs. (13) and (20)]

$$S_p = \int_0^\beta d\tau \int dx \Delta A[|\mathbf{m}(x)|^2] p_a(x)^2 - i p_a(x) B(x), \quad (\text{B1})$$

where A is a function of the superspin’s magnitude squared (for simplicity, we neglect gradient terms). In order to absorb the coefficient A , we define new momentum variables

$$p'_\alpha(x) = p_\alpha(x) \sqrt{A[|\mathbf{m}(x)|^2]}. \quad (\text{B2})$$

However, since we do not want to produce an m -dependent Jacobian, we carry out a similar transformation for the m variables as

$$m'_a(x) = m_a(x) g[|\mathbf{m}(x)|^2], \quad (\text{B3})$$

where g is chosen in order to have a Jacobian equal to 1. This requirement gives the differential equation

$$A(|\mathbf{m}|^2)^{3/2}[g(|\mathbf{m}|^2)^n - 2|\mathbf{m}|^2g(|\mathbf{m}|^2)^{n-1}g'(|\mathbf{m}|^2)] = 1, \quad (\text{B4})$$

$n (= 5)$ being the number of components of the superspin \mathbf{m} . The solution of this equation is

$$[\sqrt{r}g(r)]^n = \frac{n}{2} \int r^{n/2-1} A(r)^{-3/2} dr, \quad (\text{B5})$$

where $r = |\mathbf{m}|^2$. Upon restricting to the lowest order of Eq. (21), $A(r) = 1 + (J/2\Delta_s)r + \mathcal{O}(r^2)$, we obtain

$$g[|\mathbf{m}(x)|^2] \approx \left(1 - \frac{3J}{7\Delta_s} |\mathbf{m}(x)|^2\right), \quad (\text{B6})$$

and its inverse Eq. (23).

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- ¹S.-C. Zhang, *Science* **275**, 1089 (1997).
- ²W. Hanke, R. Eder, E. Arrigoni, A. Dorneich, S. Meixner, and M. G. Zacher, in *Festkörper Probleme/Advances in Solid State Physics*, edited by B. Kramer (Vieweg, Braunschweig, 1999), Vol. 38.
- ³W. Hanke, R. Eder, E. Arrigoni, A. Dorneich, and M. G. Zacher, *Physica C* **317**, 175 (1999).
- ⁴R. Eder, W. Hanke, and S.-C. Zhang, *Phys. Rev. B* **57**, 13 781 (1998).
- ⁵S. Rabello, H. Kohno, E. Demler, and S.-C. Zhang, *Phys. Rev. Lett.* **80**, 3586 (1998).
- ⁶C. L. Henley, *Phys. Rev. Lett.* **80**, 3590 (1998).
- ⁷D. Scalapino, S.-C. Zhang, and W. Hanke, *Phys. Rev. B* **58**, 443 (1998).
- ⁸M. Greiter, *Phys. Rev. Lett.* **79**, 4898 (1997).
- ⁹G. Baskaran and P. W. Anderson, *J. Phys. Chem. Solids* **59**, 1780 (1998).
- ¹⁰C. P. Burgess, J. M. Cline, R. MacKenzie, and R. Ray, *Phys. Rev. B* **57**, 8549 (1998).
- ¹¹C. P. Burgess and C. A. Lutken, *Phys. Rev. B* **57**, 8642 (1998).
- ¹²E. Arrigoni and W. Hanke, *Phys. Rev. Lett.* **82**, 2115 (1999).
- ¹³H.-H. Lin, L. Balents, and M. P. A. Fisher, *Phys. Rev. B* **58**, 1794 (1998).
- ¹⁴S.-C. Zhang, J.-P. Hu, E. Arrigoni, W. Hanke, and A. Auerbach, *Phys. Rev. B* **60**, 13 070 (1999).
- ¹⁵M. G. Zacher, W. Hanke, E. Arrigoni, and S.-C. Zhang, *Phys. Rev. Lett.* **85**, 824 (2000).
- ¹⁶W. Hanke, M. G. Zacher, E. Arrigoni, and S.-C. Zhang, *Physica B* **280**, 184 (2000).
- ¹⁷F. Ronning, C. Kim, D. L. Feng, D. S. Marshall, A. G. Loeser, L. L. Miller, J. N. Eckstein, I. Bozovic, and Z.-X. Shen, *Science* **282**, 2067 (1998).
- ¹⁸S. Murakami and N. Nagaosa, *J. Phys. Soc. Jpn.* **69**, 2395 (2000).
- ¹⁹J.-P. Hu and S.-C. Zhang, cond-mat/0005334, Proceedings of the MS2 Conference, Houston [Physica C (to be published)].
- ²⁰J. M. Kosterlitz, D. R. Nelson, and M. E. Fisher, *Phys. Rev. B* **13**, 412 (1976).
- ²¹D. P. Arovas, A. J. Berlinsky, C. Kallin, and S.-C. Zhang, *Phys. Rev. Lett.* **79**, 2871 (1997).
- ²²A similar action, obtained from an effective SO(5) symmetric fermionic model, has been obtained in Ref. 10. However, the Hubbard gap is not taken into account there.
- ²³R. Eder, A. Dorneich, M. G. Zacher, W. Hanke, and S.-C. Zhang, *Phys. Rev. B* **59**, 561 (1999).
- ²⁴N. Read and D. Newns, *J. Phys. C* **18**, 2651 (1985).
- ²⁵One should be aware of the fact that it is not completely correct to take the continuum limit in the functional integral at the outset (see Refs. 42–44. Different procedures for taking this limit may lead to a different value of the constraint [the “1” in Eq. (16)], which is thus not well defined in the continuum limit. However, for low-energy properties we are interested in, the precise value of the constraint is not important.
- ²⁶Due to Eq. (15), the magnitude of the superspin, rather than being constant, must be smaller than a constant.
- ²⁷F. J. Wegner, *Eur. Phys. J. B* **14**, 11 (2000).
- ²⁸D. R. Nelson, J. M. Kosterlitz, and M. E. Fisher, *Phys. Rev. Lett.* **33**, 813 (1974).
- ²⁹F. J. Wegner, *Phys. Rev. B* **6**, 1891 (1972).
- ³⁰M. E. Fisher and P. Pfeuty, *Phys. Rev. B* **6**, 1889 (1972).
- ³¹I. J. Ketley and D. J. Wallace, *J. Phys. A* **6**, 1667 (1973).
- ³²A. Aharony, *Phys. Rev. B* **8**, 4270 (1973).
- ³³R. A. Pelcovitis and D. R. Nelson, *Phys. Lett. A* **57**, 23 (1976).
- ³⁴A. Kawamoto, K. Miyagawa, Y. Nakazawa, and K. Kanoda, *Phys. Rev. B* **52**, 15 522 (1995).
- ³⁵A. Kawamoto, K. Miyagawa, and K. Kanoda, *Phys. Rev. B* **55**, 14 140 (1997).
- ³⁶It should be noted that dynamical criticality is *not* described by an SO(5)-symmetric Hamiltonian, in contrast to equilibrium criticality discussed here. This is due fact that one must include the terms Eq. (13) in order to study dynamical critical phenomena.
- ³⁷X. Hu, T. Koyama, and M. Tachiki, *Phys. Rev. Lett.* **82**, 2568 (1999).
- ³⁸X. Hu, cond-mat/9906237 (unpublished).
- ³⁹The effect of the c -axis anisotropy of the high- T_c superconductors can be taken into account by a scale transformation in the $z(c)$ direction, i.e., by transforming to the variable $z' = \chi z$ with $\chi^2 = J_{xy}a^2/J_zc^2 > 1$, where J_{xy} (J_z) is the value of J in the ab plane (c plane) (we assume that the ratio χ is the same for the AF and for the SC order parameter), and c is the lattice spacing in the z direction. The effect of the transformation can then be reabsorbed by changing $\mathcal{V} \rightarrow \mathcal{V}\chi$ in the expressions Eq. (25). This transformation implies that the correlation length in the z direction will be reduced by a factor χ^{-1} with respect to the one in the xy direction.
- ⁴⁰P. C. Hohenberg and B. I. Halperin, *Rev. Mod. Phys.* **49**, 435 (1977).
- ⁴¹J. A. Hertz, *Phys. Rev. B* **14**, 1165 (1976).
- ⁴²E. Arrigoni and G. C. Strinati, *Phys. Rev. Lett.* **71**, 3178 (1993).
- ⁴³E. Arrigoni, C. Castellani, M. Grilli, R. Raimondi, and G. C. Strinati, *Phys. Rep.* **241**, 291 (1994).
- ⁴⁴E. Arrigoni and G. C. Strinati, *Phys. Rev. B* **52**, 2428 (1995).