Instability of the O(5) multicritical behavior in the SO(5) theory of high-$T_c$ superconductors.

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Abstract

We study the nature of the multicritical point in the three-dimensional $O(3) \oplus O(2)$ symmetric Landau-Ginzburg-Wilson theory, which describes the competition of two order parameters that are $O(3)$ and $O(2)$ symmetric, respectively. This study is relevant for the $SO(5)$ theory of high-$T_c$ superconductors, which predicts the existence of a multicritical point in the temperature-doping phase diagram, where the antiferromagnetic and superconducting transition lines meet.

We investigate whether the $O(3) \oplus O(2)$ symmetry gets effectively enlarged to $O(5)$ approaching the multicritical point. For this purpose, we study the stability of the $O(5)$ fixed point. By means of a Monte Carlo simulation, we show that the $O(5)$ fixed point is unstable with respect to the spin-4 quartic perturbation with the crossover exponent $\phi_{4,4} = 0.180(15)$, in substantial agreement with recent field-theoretical results. This estimate is much larger than the one-loop $\epsilon$-expansion estimate $\phi_{4,4} = 1/26$, which has often been used in the literature to discuss the multicritical behavior within the $SO(5)$ theory. Therefore, no symmetry enlargement is generically expected at the multicritical transition.

We also perform a five-loop field-theoretical analysis of the renormalization-group flow. It shows that bicritical systems are not in the attraction domain of the stable decoupled fixed point. Thus, in these systems—high-$T_c$ cuprates should belong to this class—the multicritical point corresponds to a first-order transition.

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I. INTRODUCTION

Multicritical phenomena arise from the competition of distinct types of order. More specifically, a multicritical point (MCP) is observed at the intersection of two critical lines characterized by different order parameters. MCPs are expected in the temperature-doping phase diagram of high-$T_c$ superconductors, since, at low temperatures, these materials exhibit both superconductivity and antiferromagnetism depending on doping. The SO(5) theory attempts to provide a unified description of these two phenomena by introducing a three-component antiferromagnetic order parameter and a $d$-wave superconducting complex order parameter. This theory predicts a MCP in the temperature-doping phase diagram where the two order parameters become both critical.

Neglecting the fluctuations of the magnetic field and the quenched randomness introduced by doping—see, e.g., Ref. 7 for a critical discussion of this point—the critical behavior at the MCP is determined by the $O(3) \oplus O(2)$-symmetric Landau-Ginzburg-Wilson (LGW) Hamiltonian, given by

$$H = \int d^d x \left[ \frac{1}{2} (\partial_\mu \phi)^2 + \frac{1}{2} (\partial_\mu \psi)^2 + \frac{1}{2} r_\phi \phi^2 + \frac{1}{2} r_\psi \psi^2 + \frac{1}{24} u_0 (\phi^2)^2 + \frac{1}{24} v_0 (\psi^2)^2 + \frac{1}{4} w_0 \phi^2 \psi^2 \right], \quad (1.1)$$

where $\phi$ and $\psi$ are respectively three- and two-component real fields, associated with the antiferromagnetic and superconducting order parameters, respectively. The critical behavior at the MCP is determined by the stable fixed point (FP) of the renormalization-group (RG) flow when both $r_\phi$ and $r_\psi$ are tuned to their critical value. An interesting possibility, put forward in Refs. 5, 6, 8, 9, is that the $O(3) \oplus O(2)$ symmetry gets effectively enlarged to $O(5)$ when approaching the MCP. This requires the stability of the $O(5)$ FP in the theory (1.1).

Cuprates have a pronounced two-dimensional layer structure with relatively weak couplings between adjacent CuO$_2$ planes, so that two- and three-dimensional models should represent two extreme conditions for the possible range of properties of real high-$T_c$ superconductors, see, e.g., Ref. 14. In this paper we investigate the stability properties of the $O(5)$ FP in the three-dimensional (3-d) multicritical theory (1.1).

The phase diagram of the model with Hamiltonian (1.1) has been investigated within the mean-field approximation in Ref. 1 (see also Ref. 13). This analysis predicts the existence of a bicritical or tetracritical point. The nature of the MCP depends on the sign of the quantity $\Delta_0 \equiv u_0 v_0 - 9 w_0^2$: If $\Delta_0 > 0$ the MCP is tetracritical as in Fig. 1, while for $\Delta_0 < 0$ it is bicritical, as in Fig. 2.

The nature of the MCP in the $O(3) \oplus O(2)$ LGW theory has been extensively studied. In Refs. 5, 8, 9, it was speculated that the MCP is $O(5)$-symmetric. In three dimensions, this picture is supported by Monte Carlo (MC) simulations of a five-component $O(3) \oplus O(2)$-symmetric spin model$^9$ and by a MC study of the quantum projected SO(5) model.$^{15}$ These numerical studies showed that, within the parameter ranges considered, the scaling behavior at the MCP is consistent with an $O(5)$-symmetric critical behavior. On the other hand, the one-loop $\epsilon$-expansion results of Ref. 3 show that the $O(5)$ FP is unstable. Within this approximation, the stable FP is the biconal FP, which has only $O(3) \oplus O(2)$ symmetry.

The 3-d RG flow of $O(n_1) \oplus O(n_2)$ symmetric LGW theories for generic $n_1$ and $n_2$ was investigated within the $\epsilon$ expansion to five loops.$^4$ This analysis showed that the $O(5)$ FP and the biconal FP are both unstable. The stable FP is the decoupled FP (DFP) corresponding
FIG. 1. Phase diagram with a tetracritical point. Here, $T$ is the temperature and $g$ a second relevant parameter.

to a multicritical behavior in which the two order parameters $\phi$ and $\psi$ are effectively uncoupled. The stability of the DFP can be proved by nonperturbative arguments.\cite{16,7} Indeed, the RG dimension $y_w$ of the operator $\phi^2\psi^2$ that couples the two order parameters is given by

$$y_w = \frac{1}{\nu_{O(3)}} + \frac{1}{\nu_{O(2)}} - 3,$$

(1.2)

where $\nu_{O(3)}$ and $\nu_{O(2)}$ are the critical exponents of the O(3) and O(2) universality classes. Using\cite{17,18} $\nu_{O(3)} = 0.7112(5)$ and $\nu_{O(2)} = 0.67155(27)$, one finds $y_w = -0.1048(12)$. Note also that the MCP described by the DFP is always tetracritical, as in Fig. 1. No other stable FP is found within the $\epsilon$ expansion for the O(3)$\oplus$O(2) theory (1.1).\cite{4,19} According to these RG results, the asymptotic approach to the MCP within the SO(5) theory must be characterized by a decoupled tetracritical behavior or by a first-order transition if the system is outside the attraction domain of the DFP.

The analysis of Ref. 4 indicates that the O(5) symmetry can be asymptotically realized only by tuning an additional relevant parameter, beside the double tuning required to approach the MCP. Of course, if the system parameters are close to those needed to obtain an O(5) MCP, one observes a crossover from the O(5) behavior to the asymptotic one, which could be a decoupled critical behavior or a first-order transition. This crossover can be described in terms of universal scaling functions determined by the O(5) FP. For instance, if $T_{O(5)}$ is the critical temperature of the O(5) MCP, $g_2$ and $g_4$ are scaling fields (functions of the system parameters) associated with the two relevant perturbations of the O(5) FP such that $g_2 = g_4 = 0$ at the O(5) MCP, then the singular part of the free energy can be written as

$$F_{\text{sing}} = t^{d\nu} f(g_2 t^{-\phi_{2,2}}, g_4 t^{-\phi_{4,4}}),$$

(1.3)

where $t = (T - T_{O(5)})/T_{O(5)}$ is the reduced temperature. Here $\nu$ is the O(5) correlation-length exponent, $\phi_{2,2} > 0$ and $\phi_{4,4} > 0$ are the crossover exponents associated with the two
relevant perturbations $g_2$ and $g_4$, which are determined by the O(5) FP itself.

It has been noted\cite{16,15,14} that the crossover exponent $\phi_{4,4}$ associated with this additional

instability of the O(5) FP is rather small. This may partially explain the apparent O(5)
multicritical behavior observed in Refs. 9, 15: The MC simulations are still probing a region
in which the crossover towards the asymptotic critical behavior is so slow to be undetectable.

Within the $\epsilon$ expansion, one finds $\phi_{4,4} = \frac{1}{26} \epsilon + O(\epsilon^2)$. Using the value suggested by setting

$\epsilon = 1$, i.e. $\phi_{4,4} \approx 1/26 = 0.038...$, the authors of Refs. 15, 14 argued that any significant
deviation away from the O(5)-symmetric FP can be observed in experiments and realistic MC
simulations only when the reduced temperature is $t_{\text{cross}} \approx 10^{-10}$, making the departure away
from the O(5) symmetric point practically unobservable. On the other hand, the analysis
of the perturbative expansions in two different schemes, the 3-$d$ massive zero-momentum
scheme (six loops) and the $\epsilon$ expansion (five loops), gives a much larger estimate of $\phi_{4,4}$,\cite{4}

$\phi_{4,4} \approx 0.15$, which makes the statement of Refs. 15, 14 on the effective relevance of the O(5)

FP very questionable.\cite{4}

In this paper we return to the issue of the stability of the O(5) FP. We compute the
crossover exponent $\phi_{4,4}$ using lattice techniques based on MC simulations. We obtain $\phi_{4,4} = 0.180(15)$. This result is slightly larger than the field-theoretical (FT) ones reported in Ref. 4

and fully confirms the fact that the naive application of the one-loop $\epsilon$-expansion result gives

an estimate that is unrealistically small. Moreover, we perform a detailed FT analysis of

the RG flow in the 3-$d$ scheme known as minimal-subtraction scheme without $\epsilon$ expansion.\cite{20}

We find that bicritical systems that have $\Delta_0 < 0$ never flow towards the DFP. Therefore,

these systems, which are those of interest for high-$T_c$ superconducting materials according

to the analysis of Ref. 11, should have a first-order MCP.

The paper is organized as follows. In Sec. II we discuss the stability of the O(5) FP and

present a MC determination of the crossover exponent $\phi_{4,4}$. In Sec. III we discuss the RG

flow and determine the attraction domain of the DFP. In Sec. IV we report our conclusions.
The five-loop perturbative series used in Sec. III to determine the RG flow are reported in the appendix.

II. STABILITY OF THE O(5) FIXED POINT

A. General considerations

In order to determine the stability properties of the O(5) FP, we must determine the RG dimensions of the perturbations present in the Hamiltonian (1.1) that break the O(5) symmetry down to O(3) ⊕ O(2). They can be expressed in terms of homogeneous polynomials of the fields $P_{ml}$, where $m$ is the power of the fields and $l$ the spin of the representation of the O(5) group. The classification in terms of spin values is particularly convenient, since polynomials with different spin do not mix under RG transformations and the RG dimension $y_{ml}$ does not depend on the particular component of the spin-$l$ representation. We refer to Ref. 4 for details. For $m = 2$ (resp. 4), the only possible values of $l$ are $l = 0, 2$ (resp. $l = 0, 2, 4$). Explicitly, we define

$$P_{2,0} = \frac{1}{2} (\phi^2 + \psi^2),$$
$$P_{2,2} = \frac{2}{5} \phi^2 - \frac{3}{2} \psi^2,$$
$$P_{4,0} = P_{2,0}^2,$$
$$P_{4,2} = P_{2,0} P_{2,2},$$
$$P_{4,4} = \frac{40}{63} \phi^2 \psi^2 - \frac{5}{21} (\psi^2)^2 - \frac{8}{63} (\phi^2)^2. \hspace{1cm} (2.1)$$

Note that in general all these operators renormalize multiplicatively except $P_{4,2}$ that may mix with the lower-dimensional operator $P_{2,2}$.

Hamiltonian (1.1) can be rewritten in the form

$$\mathcal{H} = \int d^d x \left[ \frac{1}{2} (\partial_\mu \phi)^2 + \frac{1}{2} (\partial_\mu \psi)^2 + \frac{1}{2} (r_0 P_{2,0} + r_2 P_{2,2})^2 + \frac{1}{24} (f_{0,0} P_{4,0} + f_{2,0} P_{4,2} + f_{4,0} P_{4,4}) \right], \hspace{1cm} (2.2)$$

where

$$f_{0,0} = \frac{4}{35} (15 u_0 + 8 v_0 + 36 w_0),$$
$$f_{2,0} = \frac{4}{9} (5 u_0 - 4 v_0 - 3 w_0),$$
$$f_{4,0} = 6 w_0 - u_0 - v_0. \hspace{1cm} (2.3)$$

If $r_2 = f_{2,0} = f_{4,0} = 0$ we obtain the O(5)-invariant Hamiltonian.

The RG dimensions of the relevant quadratic perturbations $P_{2,0}$ and $P_{2,2}$ are respectively \(^{21,4,22,23}\) $y_{2,0} = 1/\nu = 1.31(1)$ ($\nu$ is the O(5) critical exponent associated with the correlation length) and $y_{2,2} = 1.83(1)$. The corresponding crossover exponents are $\phi_{2,0} = 1$ and $\phi_{2,2} = y_{2,2} \nu = 1.40(2)$. The corresponding Hamiltonian parameters $r_{\phi}$ and $r_{\psi}$ must be tuned to approach the MCP. The spin-0 quartic perturbation $P_{4,0}$ determines the leading
scaling corrections in the $O(5)$ vector model; its RG dimension is $y_{4,0} = -0.79(2)$.\textsuperscript{4} The spin-2 quartic perturbation $P_{4,2}$ turns out to be irrelevant: $y_{4,2} = -0.441(13)$.\textsuperscript{4} The $O(5)$ FP is also unstable with respect to the perturbation $P_{4,4}$ (more generally, the $O(N)$ FP is unstable against the spin-4 quartic perturbation for $N > N_c$ with $N_c \lesssim 3$, see Refs. 24–27). The corresponding RG dimension $y_{4,4}$ is given by $y_{4,4} = \frac{1}{12} \epsilon + O(\epsilon^2)$ close to four dimensions. A naive extrapolation of this result to three dimensions, achieved by setting $\epsilon = 1$, suggests a very small value. On the other hand,\textsuperscript{27,4,23} a six-loop analysis of the 3-d perturbative series in the massive zero-momentum scheme gives $y_{4,4} = 0.189(10)$, while the five-loop $\epsilon$ expansion gives $y_{4,4} = 0.198(11)$. These estimates are still moderately small, though much larger than the estimate $y_{4,4} = 1/13$ obtained by naively setting $\epsilon = 1$ in the one-loop $\epsilon$-expansion result.

B. Monte Carlo determination of the critical exponent $y_{4,4}$

In the following we present a MC calculation of the RG dimension $y_{4,4}$ and of the crossover exponent $\phi_{4,4} \equiv \nu y_{4,4}$. As we shall see, the result will provide conclusive evidence for the fact that the 3-d exponent $\phi_{4,4}$ is actually much larger that the $O(\epsilon)$ result, in agreement with the high-order FT analyses.

We consider the 5-vector model on a simple cubic lattice of size $L^3$ with Hamiltonian

$$\mathcal{H} = -\beta \sum_{\langle xy \rangle} \vec{s}_x \cdot \vec{s}_y,$$

(2.4)

where $\vec{s}_x$ is a five-component unit vector, and the summation is extended over all nearest-neighbor pairs $\langle xy \rangle$. The RG dimension $y_{4,4}$ can be obtained by studying the scaling behavior of the cubic-symmetric perturbation

$$P_c = \sum_x \sum_{i=1}^5 s^4_{x,i}$$

(2.5)

at the critical point. Indeed, the operator $P_c$ is a particular combination of the spin-4 and spin-0 operators\textsuperscript{4} and thus its scaling behavior allows the determination of $y_{4,4}$ (assuming of course that $y_{4,0} < y_{4,4}$). We follow closely Ref. 26 where $y_{4,4}$ was computed in the $N$-vector model for $N = 2, 3, \text{and} 4$. We define

$$\vec{M} \equiv \sum_x \vec{s}_x, \quad R = \frac{\sum_{i=1}^5 M_i^4}{(M^2)^2},$$

(2.6)

and compute the correlation

$$D_R \equiv \langle RP_c \rangle - \langle R \rangle \langle P_c \rangle.$$

(2.7)

The RG dimension $y_{4,4}$ is obtained from the finite-size scaling behavior of $D_R$ at the critical point, since

$$D_R(L, \beta = \beta_c) \sim L^{y_{4,4}}$$

(2.8)
for $L \to \infty$.

In our simulations we used combinations of wall-cluster, single-cluster, and overrelaxation updates. In order to determine the critical point and the standard critical exponents, we considered lattices of size $L \leq 128$ for several values of $\beta$ close to 1.1813. We measured the Binder cumulant

$$U_4 = \frac{\langle (\vec{M}^2)^2 \rangle}{\langle \vec{M}^2 \rangle^2} \quad (2.9)$$

and the ratio $Z_a/Z_p$, where $Z_p$ is the partition function with periodic boundary conditions and $Z_a$ is the partition function with periodic boundary conditions in two directions and antiperiodic boundary conditions in the third one (for a detailed discussion of this quantity see Refs. 30, 18, 17 and references therein).

The critical value $\beta_c$ is estimated by employing the standard crossing method for the Binder cumulant and for $Z_a/Z_p$. We obtain

$$\beta_c = 1.18138(3), \quad (2.10)$$

where the quoted uncertainty includes both statistical and systematic errors. It is compatible with the estimate $\beta_c = 1.18127(10)$ obtained using only lattices with $L \leq 32$, indicating that scaling corrections are quite small. The result (2.10) is consistent with the estimate obtained from the analysis of the 21st-order high-temperature expansion of the magnetic susceptibility computed in Ref. 32, but much more precise. The analysis also provides the critical values of $U_4$ and of $Z_a/Z_p$: $U_4^* = 1.069(1)$ and $(Z_a/Z_p)^* = 0.071(1)$.

We estimate the exponent $\nu$ from the $L$-dependence of the slope of $Z_a/Z_p$ and of $U_4$ along the line in the $(\beta, L)$ plane on which $Z_a/Z_p = 0.071$ (which means that, for each $L$, we take the two quantities at the value of $\beta$ where $Z_a/Z_p$ takes the value 0.071). Fitting the slope of $Z_a/Z_p$ for data with $16 \leq L \leq 128$ with a simple power-law Ansatz, we obtain $\nu = 0.7782(14)$ with $\chi^2$/d.o.f. = 0.49, where d.o.f. indicates the number of degrees of freedom of the fit. If we use the data with $8 \leq L \leq 64$ we obtain instead $\nu = 0.7766(5)$ with $\chi^2$/d.o.f. = 0.95. The systematic error due to scaling corrections should not be (much) larger than the difference between these two results. Roughly, assuming that scaling corrections are dominated by the leading one with exponent $\omega = -y_{4,0} = 0.79(2)$, the systematic error on $\nu = 0.7782(15)$ should be given approximately by $(2^\omega - 1)^{-1}$ times the difference, i.e. it should be approximately 0.002. Fitting the slope of the Binder cumulant, we obtain $\nu = 0.7809(32)$ (resp. $\nu = 0.7802(13)$) from data with $16 \leq L \leq 128$ (resp. $8 \leq L \leq 64$). These results are consistent with those from the slope of $Z_a/Z_p$ but less precise. As our final estimate we give

$$\nu = 0.779(3), \quad (2.11)$$

where the error should also include the systematic uncertainty due to scaling corrections. This estimate clearly rules out the MC result $\nu = 0.728(18)$ of Ref. 9. It is also slightly larger than the FT estimate $\nu = 0.762(7)$. Moreover, by fitting the magnetic susceptibility $\chi$ at $Z_a/Z_p = 0.071$ we find

$$\eta = 0.034(1), \quad (2.12)$$
TABLE I. Estimates of $D_R$ at $\beta = 1.18138$. The number reported in parentheses is the statistical error, while the number in brackets gives the error due to the uncertainty on the estimate of $\beta_c$.

| $L$ | $D_R$    |
|-----|---------|
| 4   | 0.023979(6)[4] |
| 5   | 0.025668(8)[6] |
| 6   | 0.026950(10)[9] |
| 7   | 0.028019(13)[10] |
| 8   | 0.028942(16)[12] |
| 9   | 0.029733(18)[15] |
| 10  | 0.030501(22)[18] |
| 11  | 0.031100(25)[22] |
| 12  | 0.031752(28)[25] |
| 14  | 0.032900(36)[31] |
| 16  | 0.033825(44)[38] |
| 18  | 0.034769(53)[47] |
| 20  | 0.035638(81)[47] |
| 22  | 0.036461(72)[60] |
| 24  | 0.037134(88)[70] |

where again the quoted error includes possible systematic errors due to scaling corrections. Performing this analysis we followed closely Refs. 30, 18, 17, where the models with 2, 3, and 4 components were studied.

The determination of $y_{4,4}$ through Eq. (2.8) requires a very large statistics, which limits us to lattices with $L \leq 24$. Typically, approximately $10^9$ measurements were performed for each lattice size. Most of the simulations were performed at $\beta = 1.18127$. In order to extrapolate the data to other values of $\beta$ and, in particular, to $\beta_c$, we also performed simulations at $\beta = 1.18$ and $\beta = 1.183$, obtaining an estimate of the derivative of $D_R$ with respect to $\beta$. In Table I we summarize the numerical results for $D_R$ at $\beta = 1.18138 \approx \beta_c$.

First, we fit these data with the simple power-law ansatz (2.8). The results are summarized in Table II. The fits are stable starting from $L_{\text{min}} = 8$. Also the $\chi^2$/d.o.f. for fits with $L_{\text{min}} \geq 8$ is smaller than one. In order to check the dependence of the result for $y_{4,4}$ on the numerical estimate of $\beta_c$, we repeat these fits using the values of $D_R$ at $\beta = 1.18135$ and $\beta = 1.18141$, which correspond to adding or subtracting one error bar to $\beta_c$. For example, for $L_{\text{min}} = 11$ we obtain the estimates $y_{4,4} = 0.2256(19)$ and $y_{4,4} = 0.2283(19)$ for $\beta = 1.18135$ and $\beta = 1.18141$, respectively. Optimistically, we could quote the final result $y_{4,4} = 0.227(3)$, where the error bar includes the statistical uncertainty as well as the error due to the uncertainty in the estimate of $\beta_c$. This estimate would be reliable if scaling corrections, and in particular the leading ones associated with the exponent $\omega = -y_{4,0} = 0.79(2)$, are suppressed. This seems to be supported by the above-reported analysis to determine $\beta_c$ and the critical exponents, where no evidence for the leading scaling corrections was found within our statistical errors.
TABLE II. Fits of $D_R(\beta = 1.18138 \approx \beta_c)$ on lattices of size $L \geq L_{\text{min}}$ with the power-law Ansatz $D_R = cL^{y_{4,4}}$. In the final column the $\chi^2$ per degree of freedom (d.o.f.) is reported.

| $L_{\text{min}}$ | $y_{4,4}$     | $c$           | $\chi^2$/d.o.f. |
|-----------------|--------------|---------------|-----------------|
| 6               | 0.2333(3)    | 0.01778(2)    | 8.30            |
| 7               | 0.2290(8)    | 0.01796(3)    | 2.20            |
| 8               | 0.2268(10)   | 0.01807(4)    | 0.93            |
| 9               | 0.2261(12)   | 0.01810(6)    | 0.92            |
| 10              | 0.2252(15)   | 0.01815(7)    | 0.90            |
| 11              | 0.2270(19)   | 0.01806(9)    | 0.60            |

In order to be conservative, we also analyze the data allowing for a nonvanishing scaling correction, i.e. we fitted our data with the ansatz

$$D_R(L, \beta = \beta_c) = cL^{y_{4,4}}(1 + c'L^{-\omega})$$

where we set $\omega = 0.79$.\textsuperscript{4} Note that the results for $y_{4,4}$ depend very little on the precise value for $\omega$. The results of the fits are summarized in Table III. Only for $L_{\text{min}} < 8$ do we get an amplitude $c'$ that is different from zero within error bars. However, for these fits also $\chi^2$/d.o.f. is large. This suggests that for the small lattice sizes $L < 8$ actually subleading scaling corrections dominate. The results for the exponent $y_{4,4}$ obtained from $L_{\text{min}} > 7$ are completely consistent with the results reported above for the power-law ansatz without corrections. However, here the error bars are considerably larger. Since we are not able to exclude leading corrections to scaling on a firm basis, we take the error resulting from the fits that include leading corrections to scaling as our final estimate. Taking into account also the uncertainty in our estimate of $\beta_c$ we arrive at the final estimate

$$y_{4,4} = 0.23(2).$$

Note that the reported error estimate is probably quite conservative. Using the estimate (2.11) of $\nu$, we obtain $\phi_{4,4} \equiv y_{4,4}\nu = 0.180(15)$ for the corresponding crossover exponent.

### III. RENORMALIZATION-GROUP FLOW

The presence of a stable FP does not imply that the MCP should always correspond to a second-order transition controlled by the stable FP. Indeed, this happens only if the system is in the attraction domain of the stable FP. It is thus of interest to determine the attraction domain of the DFP. For this purpose we study the RG flow of the system, i.e., the RG trajectories along which the quartic Hamiltonian parameters $u_0$, $v_0$, and $w_0$ are kept fixed.

We consider the flow directly in three dimensions, using the minimal-subtraction ($\overline{\text{MS}}$) scheme without $\epsilon$ expansion.\textsuperscript{20} In this scheme one considers the massless (critical) theory in dimensional regularization within the $\overline{\text{MS}}$ scheme.\textsuperscript{33} RG functions are obtained in terms of
TABLE III. Fits of $D_R(\beta = 1.18138 \approx \beta_c)$ on lattices of size $L \geq L_{\text{min}}$ with the Ansatz (2.13). The exponent $\omega$ was fixed: $\omega = 0.79$. In the final column the $\chi^2$ per degree of freedom (d.o.f.) is reported.

| $L_{\text{min}}$ | $y_{4,4}$ | $c$   | $c'$  | $\chi^2$/d.o.f. |
|------------------|----------|-------|-------|-----------------|
| 5                | 0.189(3) | 0.0208(2) | -0.321(16) | 3.02           |
| 6                | 0.199(4) | 0.0201(3) | -0.244(27) | 1.87           |
| 7                | 0.210(5) | 0.0193(3) | -0.152(37) | 1.24           |
| 8                | 0.221(8) | 0.0185(6) | -0.054(70) | 0.98           |
| 9                | 0.226(4) | 0.0181(7) | -0.001(95) | 1.06           |
| 10               | 0.245(15) | 0.0168(10) | 0.20(16) | 0.83           |
| 11               | 0.226(18) | 0.0182(13) | -0.01(20) | 0.71           |

the renormalized couplings $u, v, w$ and of $\epsilon = 4 - d$. Subsequently $\epsilon$ is set to its physical value $\epsilon = 1$, providing a 3-$d$ scheme in which the 3-$d$ RG functions are expanded in powers of the MS renormalized quartic couplings $u, v, w$. This scheme differs from the standard $\epsilon$ expansion in which one expands the RG functions in powers of $\epsilon$. The $\overline{\text{MS}}$ $\beta$ functions have been computed to five loops for generic $O(n_1) \oplus O(n_2)$ LGW theories. In the appendix we report the five-loop series that are used in this section to determine the RG flow of the $O(3) \oplus O(2)$ case.

The RG trajectories are obtained by solving the differential equations

$$
-\lambda \frac{du}{d\lambda} = \beta_u[u(\lambda), v(\lambda), w(\lambda)],
$$

$$
-\lambda \frac{dv}{d\lambda} = \beta_v[u(\lambda), v(\lambda), w(\lambda)],
$$

$$
-\lambda \frac{dw}{d\lambda} = \beta_w[u(\lambda), v(\lambda), w(\lambda)],
$$

(3.1)

with $\lambda \in [0, \infty)$ and the initial conditions

$$
\left. \frac{du}{d\lambda} \right|_{\lambda=0} = u_0, \quad \left. \frac{dv}{d\lambda} \right|_{\lambda=0} = v_0, \quad \left. \frac{dw}{d\lambda} \right|_{\lambda=0} = w_0.
$$

(3.2)

Note that the trajectories do not depend on the Hamiltonian parameters individually, but only through their dimensionless ratios. For instance, by rescaling $\lambda \rightarrow \lambda/w_0$, the initial conditions depend only on $u_0/w_0$ and $v_0/w_0$. The necessary resummation of the series is performed by employing the Padé-Borel method; see, e.g., Refs. 35, 24.

In this RG scheme the coordinates of the $O(5)$ FP are $u^* = v^* = 3w^* \approx 0.62$. Since the $O(5)$ FP has only one instability direction in the $u, v, w$ space, RG trajectories flowing to the $O(5)$ FP separate the flow into two different domains. In order to characterize these domains, we consider the dimensionless ratios $f_{2,0}/f_{0,0}, f_{4,0}/f_{0,0}$, cf. Eq. (2.3), and $\Delta_0/f_{0,0}^2$ where $\Delta_0 = u_0v_0 - 9w_0^2$. In Figs. 3 and 4 we report the initial conditions that correspond to
FIG. 3. Initial conditions for trajectories flowing to the O(5) FP in the $f_{2,0}/f_{0,0}$, $f_{4,0}/f_{0,0}$ plane.

trajectories flowing to the O(5) FP, respectively in terms of $f_{2,0}/f_{0,0}$ and $f_{4,0}/f_{0,0}$ and in terms of $\Delta_0/f_{0,0}^2$ and $f_{4,0}/f_{0,0}$. The results reported in the figures were obtained by resumming the $\beta$ functions with a [5/1] Padé-Borel approximant. We used several different values of the Borel-Leroy parameter $b$: the results are essentially independent of this parameter.

Since the spin-4 perturbation is relevant, asymptotically the RG trajectories reaching the O(5) FP lie in the plane $f_4 = 0$. One may then naively expect that the initial conditions for trajectories flowing to the O(5) FP have $f_{4,0}/f_{0,0}$ small. As it can be seen from Fig. 3 this is not really true, although $|f_{4,0}/f_{0,0}| \ll |f_{2,0}/f_{0,0}|$. We also report the results in terms of $\Delta_0/f_{0,0}^2$ for two reasons. First, $\Delta_0 \equiv u_0v_0 - 9w_0^2$ determines the nature (bicritical or tetracritical) of the phase diagram. Second, in the mean-field approximation $\Delta_0 = 0$ is required for obtaining an O(5)-invariant transition. Indeed, if one ignores fluctuations and thus neglects the kinetic term and rescales the fields as $\phi \rightarrow (\bar{u}/u_0)^{1/4}\phi$ and $\psi \rightarrow (\bar{u}/v_0)^{1/4}\psi$, one obtains an O(5)-invariant quartic potential only for $\Delta_0 = 0$. Note that, as show by Fig. 4, this mean-field condition is not actually satisfied when fluctuations are taking into account, although $\Delta_0/f_{0,0}^2$ is small whenever $f_{4,0}/f_{0,0}$ is also small.

The curve reported in Fig. 3, of equation $f_{4,0}/f_{0,0} = g(f_{2,0}/f_{0,0})$, separates the space of initial conditions into two different domains. We determine now which of them contains the attraction domain of the DFP, whose coordinates are $u^* \approx 0.688$, $v^* \approx 0.745$, $w^* = 0$, i.e., $f_0^* \approx 1.86$, $f_2^* \approx 0.204$, $f_4^* \approx -1.43$ (here, $f_i$ are the renormalized couplings related the Hamiltonian couplings $f_{i,0}$). A numerical analysis indicates that the DFP can only be reached for initial conditions that are inside the curve reported in Fig. 3, i.e., for values satisfying $f_{4,0}/f_{0,0} < g(f_{2,0}/f_{0,0})$. Points that satisfy the opposite inequality correspond to trajectories running away to infinity. These results can be rephrased in terms of $\Delta_0$. A simple calculation shows that, if $f_{4,0}/f_{0,0} < g(f_{2,0}/f_{0,0})$, then $\Delta_0 > 0$. In other words, bicritical systems correspond to trajectories running away to infinity: in this case the MCP corresponds to a first-order transition. On the other hand, tetracritical systems may show, depending on the values of the parameters, a second-order multicritical behavior controlled by the DFP or a first-order transition. Note that the first-order nature of the bicritical point should have been guessed a priori: indeed, by its very nature, the DFP can only correspond to a tetracritical phase diagram and thus cannot be relevant for bicritical systems.
FIG. 4. Initial conditions for trajectories flowing to the $O(5)$ FP in the $f_{4,0}/f_{0,0}$, $\Delta_0/f_{0,0}^2$ plane. Points belonging to the lower dashed curve have $f_{2,0}/f_{0,0} > 0$, those belonging to the upper continuous one have $f_{2,0}/f_{0,0} < 0$.

IV. CONCLUSIONS

In conclusion, our MC simulations confirm that the $O(5)$ FP is unstable in the 3-d $O(3)\oplus O(2)$ LGW theory. The instability of the $O(5)$ FP is related to the presence of the spin-4 quartic perturbation in the $O(3)\oplus O(2)$ LGW Hamiltonian. We obtain an accurate estimate of its RG dimension, $y_{4,4} = 0.23(2)$, and of the corresponding crossover exponent, $\phi_{4,4} \equiv y_{4,4}\nu = 0.180(15)$. These results are slightly larger than, but in substantial agreement with, the FT results. The only stable FP of the $O(3)\oplus O(2)$ LGW theory is the DFP.

Therefore, if the system is in its attraction domain, a decoupled critical behavior should be observed at the MCP, with a tetracritical phase diagram.

As argued in Refs. 8, 14, sufficiently close to the MCP, the $O(3)\oplus O(2)$ LGW Hamiltonian is the effective theory of a realistic SO(5) theory of high-$T_c$ superconductors, such as the projected SO(5) model. The calculations of Ref. 11 indicate that realistic models have a bicritical phase diagram with $\Delta_0 < 0$. Therefore, the analysis that we have reported indicates that the MCP should correspond to a first-order transition and the phase diagram should be like that reported in Fig. 5. Note that first-order transitions should also be observed along the $O(2)$ and $O(3)$ lines close to the MCP. Therefore, the $O(2)$ and $O(3)$ lines in the temperature-doping phase diagram are expected to present, starting from the MCP, first-order transitions up to a tricritical point with an essentially mean-field critical behavior (apart from logarithms), and then second-order transitions in the $O(2)$ and $O(3)$ universality class, respectively.

As put forward in Refs. 16, 15, 14, an effective $O(5)$ multicritical behavior may still be observed in a preasymptotic region when the effective breaking of the $O(5)$ symmetry, and in particular its spin-4 component, is small. The observation was essentially based on the value of the crossover exponent suggested by an $O(\epsilon)$ calculation, i.e. $\phi_{4,4} = \epsilon/26$, which gives $\phi_{4,4} \simeq 0.038$ when one sets $\epsilon = 1$. Using this estimate of $\phi_{4,4}$, the authors of Refs. 15, 14 argued that significant deviations from the symmetric $O(5)$ multicritical behavior cannot be observed in experiments and realistic MC simulations, since the crossover to the eventual
asymptotic behavior is expected only when the reduced temperature is $t_{\text{cross}} \approx 10^{-10}, 10^{-11}$. On the other hand, as shown in this paper, the actual 3-d value of $\phi_{4,4}$ is much larger. Taking for granted the arguments leading to the estimate $t_{\text{cross}} \approx 10^{-10}$, one can easily see that, using the actual value of $\phi_{4,4}$, the crossover reduced temperature $t_{\text{cross}}$ would change from $10^{-10}$ to $36 t_{\text{cross}} \approx 10^{-2}$. Taking into account that this is a very rough estimate, which may easily miss one order of magnitude, we conclude that the actual 3-d value $\phi_{4,4} \approx 0.18$ is sufficiently large to give rise to observable crossover effects towards the real asymptotic behavior even in systems with a moderately small breaking of the O(5) symmetry, such as the projected SO(5) model. These crossover effects should be observable without the need of reaching extremely small values of the reduced temperature, as argued in Refs. 14, 15.

We would also like to stress that the value $\phi_{4,4} \approx 0.18$ is of the same order of magnitude of the crossover exponent appearing in other physical systems. For instance, in randomly dilute uniaxial magnetic materials, see, e.g., Refs. 24, 37, the pure Ising FP is unstable with a crossover exponent $\phi \approx 0.11$, which is substantially smaller than $\phi_{4,4}$ at the O(5) FP. In these systems the asymptotic critical behavior has been precisely observed both numerically and experimentally, and sizeable crossover effects from the Ising to the random-exchange critical behavior have been observed also in the case of small dilution, without the need of reaching extremely small reduced-temperature values.

Since we have computed the initial conditions that guarantee the flow to reach the O(5) FP, we can try to understand more quantitatively the behavior of the model discussed in Ref. 11. Using their notations, at the classical level the projected SO(5) model is equivalent to the LGW theory with

$$\frac{f_{2,0}}{f_{0,0}} = \frac{5(\eta^2 - 1)}{2(2 + 3\eta^2)}, \quad \frac{f_{4,0}}{f_{0,0}} = 0,$$

Fig. 5. Phase diagram with a first-order bicritical point. Here, $T$ is the temperature and $g$ a second relevant parameter. The thick lines correspond to first-order transitions.
where $\eta$ is related to the different mobilities of the holes and of the magnons. The model is SO(5) invariant for $\eta = 1$ as expected. As $\eta$ decreases (a realistic value would be $15 \eta^2 = 0.225$), $f_{2,0}/f_{0,0}$ becomes negative and increases in absolute value. Comparing with Fig. 3, we see that the SO(5) breaking effects increase. An estimate of the crossover temperature $t_{\text{cross}}$ can be obtained by requiring $\delta t^{-\phi_{\nu,4}} \sim 1$, where $\delta$ somehow measures the distance between the initial condition and the line corresponding to the O(5) invariant models. In this case, we can take $\delta = |f_{2,0}/f_{0,0}|$ and thus estimate $t_{\text{cross}} \sim 10^{-1}$ for the realistic case $15 \eta^2 = 0.225$. Note that $t_{\text{cross}}$ decreases rapidly with increasing $\eta$ and indeed one obtains $t_{\text{cross}} \sim 10^{-3}$ for the model studied numerically ($\eta^2 = 1/2$) in Ref. 15, thereby explaining the apparent O(5) behavior that was observed. Inclusion of the quantum corrections has the effect of increasing the SO(5) breaking. For instance, for $\eta^2 = 0.225$ we have

$$f_{2,0} = -0.724 - 4.36\kappa, \quad f_{4,0} = 1.26\kappa,$$

(4.2)

where $\kappa = \mathcal{D}J_{I_s}$ (see Ref. 11 for the definitions) is a positive quantity. Thus, for the realistic case, the initial conditions are pushed even further from the line corresponding to the O(5) invariant models.

**APPENDIX A: THE FIVE-LOOP SERIES OF THE $\beta$ FUNCTIONS IN THE $\overline{\text{MS}}$ SCHEME**

The expansion of the $\beta$ functions of generic $O(n_1) \oplus O(n_2)$ LGW theories in the modified minimal-subtraction ($\overline{\text{MS}}$) renormalization scheme is known to five loops.\(^4\) In Ref. 4 only the $\epsilon$ expansions of some exponents were reported. Here we report the five-loop series of the $\beta$ functions of the $O(3) \oplus O(2)$ LGW theory (1.1) in powers of the $\overline{\text{MS}}$ renormalized quartic couplings.

In order to renormalize the $O(3) \oplus O(2)$ LGW theory (1.1) in the $\overline{\text{MS}}$ scheme, one sets $\phi = Z^{1/2}_{\phi_r}$, $\varphi = Z^{1/2}_{\varphi_r}$, $u_0 = A_d\mu^\epsilon Z_u(u,v,w)$, $v_0 = A_d\mu^\epsilon Z_v(u,v,w)$, $w_0 = A_d\mu^\epsilon Z_w(u,v,w)$, where $u,v,w$ are the $\overline{\text{MS}}$ renormalized quartic couplings. The renormalization functions $Z_{\phi,\varphi}$ and $Z_{u,v,w}$ are normalized so that $Z_{\phi,\varphi} \approx 1$ and $Z_{u,v,w} \approx u,v,w$ at tree level. Here $A_d$ is a $d$-dependent constant given by $A_d \equiv 2^{d-1}\pi^{d/2}(d/2)$. The $\overline{\text{MS}}$ $\beta$ functions $\beta_{u,v,w}$ are obtained by differentiating the renormalized couplings with respect to the scale $\mu$, keeping the bare couplings $u_0$, $v_0$, $w_0$ fixed. The $O(3) \oplus O(2)$ $\beta$ functions are given by

\[
\begin{align*}
\beta_u &= (d - 4)u + \frac{11}{6}u^2 + 3w^2 - \frac{23}{12}u^3 - \frac{5}{2}uw^2 - 6w^3 + \sum_{ijk} b_{ijk}^{(u)}u^i v^j w^k, \\
\beta_v &= (d - 4)v + \frac{5}{3}v^2 + \frac{9}{2}w^2 - \frac{5}{3}v^3 - \frac{15}{4}vw^2 - 9w^3 + \sum_{ijk} b_{ijk}^{(v)}u^i v^j w^k, \\
\beta_w &= (d - 4)w + \frac{5}{6}uw + \frac{2}{3}vw + 2w^2 - \frac{25}{72}u^2 w - \frac{5}{2}uw^2 - \frac{5}{18}v^2 w - 2vw^2 - \frac{21}{8}w^3 + \sum_{ijk} b_{ijk}^{(w)}u^i v^j w^k.
\end{align*}
\]
The coefficients $b_{ijk}^{(u,v,w)}$ up to five loops, i.e. for $4 \leq i + j + k \leq 6$, are reported in Tables IV. In order to save space, we report them numerically, although we have their exact expressions in terms of fractions and of $\zeta$ functions with integer argument.
| $i, j, k$ | $b_{ijk}^{(u)}$ | $b_{ijk}^{(v)}$ | $b_{ijk}^{(w)}$ |
|----------|----------------|----------------|----------------|
| 4,0,0    | 5.95643        | 0              | 0              |
| 3,1,0    | 0              | 0              | 0              |
| 3,0,1    | 0              | 0              | 0.902778       |
| 2,2,0    | 0              | 0              | 0              |
| 2,1,1    | 2.21875        | 0.234375       | 4.44611        |
| 2,0,2    | 0              | 0              | 0              |
| 1,3,0    | 0              | 0              | 0              |
| 1,2,1    | 0.125          | 3.46875        | 3.50134        |
| 1,1,2    | 0              | 54.262         | 11.6624        |
| 1,0,3    | 38.6747        | 15             | 14.0051        |
| 0,4,0    | 0              | 4.99347        | 0              |
| 0,3,1    | 0              | 0.652778       | 0              |
| 0,2,2    | 0.125          | 3.46875        | 3.50134        |
| 0,1,3    | 8              | 54.262         | 11.6624        |
| 0,0,4    | 13.9123        | 20.4465        | 12.8874        |
| 5,0,0    | −27.3529       | 0              | 0              |
| 4,1,0    | 0              | 0              | 0              |
| 4,0,1    | 0              | 0              | −2.91484       |
| 3,2,0    | 0              | 0              | 0              |
| 3,1,1    | 0              | 0              | 0              |
| 3,0,2    | −5.56225       | −1.0098        | −17.0442       |
| 2,3,0    | 0              | 0              | 0              |
| 2,2,1    | 1.18623        | −0.0839266     | −2.56238       |
| 2,0,3    | −188.898       | −21.3002       | −51.1747       |
| 1,4,0    | 0              | 0              | 0              |
| 1,3,1    | 0              | 0              | 0              |
| 1,2,2    | −0.144409      | 1.81816        | −2.57945       |
| 1,1,3    | −19.1406       | −34.1777       | −41.1293       |
| 1,0,4    | −173.188       | −169.835       | −108.727       |
| 0,5,0    | 0              | −21.9072       | 0              |
| 0,4,1    | 0              | 0              | −1.99192       |
| 0,3,2    | −0.489598      | −7.99393       | 12.3167        |
| 0,2,3    | −10.9914       | −247.731       | −39.1403       |
| 0,1,4    | −91.5308       | −239.138       | −94.7246       |
| 0,0,5    | −120.043       | −191.964       | −100.117       |
| 6,0,0    | 156.207        | 0              | 0              |
| 5,1,0    | 0              | 0              | 0              |
| 5,0,1    | 0              | 0              | 12.3408        |
| 4,2,0    | 0              | 0              | 0              |
| 4,1,1    | 0              | 0              | 0              |
| 4,0,2    | 6.47354        | 2.81164        | 80.795         |
| 3,3,0    | 0              | 0              | 0              |
| 3,2,1    | 0              | 0              | 0              |
| 3,1,2    | 2.43996        | −0.068611      | 11.0339        |
| 3,0,3    | 1146.82        | 77.9976        | 249.36         |
| 2,4,0    | 0              | 0              | 0              |
| 2,3,1    | 0              | 0              | 0              |
| 2,2,2    | 1.98376        | 3.09444        | 5.96446        |
| 2,1,3    | 35.922         | 57.0315        | 124.802        |
| 2,0,4    | 1294.73        | 518.911        | 617.85         |
| 1,5,0    | 0              | 0              | 0              |
| 1,4,1    | 0              | 0              | 0              |
| 1,3,2    | −0.142137      | 4.13976        | 9.84045        |
| 1,2,3    | 34.0863        | 66.1707        | 119.023        |
| 1,1,4    | 659.256        | 1136.61        | 636.697        |
| 1,0,5    | 1776.58        | 1751.3         | 1155.64        |
| 0,6,0    | 0              | 120.141        | 0              |
| 0,5,1    | 0              | 0              | 7.99517        |
| 0,4,2    | 1.27762        | 10.0207        | 54.8793        |
| 0,3,3    | 37.2454        | 1426.49        | 178.161        |
| 0,2,4    | 257.6          | 1657.51        | 434.147        |
| 0,1,5    | 943.812        | 2594.22        | 1031.67        |
| 0,0,6    | 1108.93        | 1879.79        | 852.872        |
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