Phase Diagram of the Two-Channel Kondo Lattice

Mark Jarrell,[1] Hanbin Pang,[1] and D. L. Cox[2]
[1]*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221*
[2]*Department of Physics, The Ohio State University, Columbus, Ohio 43202*
(Received 20 September 1996)

The phase diagram of the two-channel Kondo lattice model is examined with a quantum Monte Carlo simulation in the limit of infinite dimensions. Commensurate (and incommensurate) antiferromagnetic and superconducting states are found. The antiferromagnetic transition is very weak and continuous. The superconducting transition is discontinuous to an odd-frequency channel-singlet and spin-singlet pairing state. [S0031-9007(97)02626-4]

PACS numbers: 75.30.Mb, 71.27.+a, 75.10.Dg

Despite strong local Coulomb correlations and a huge electronic effective mass (100–1000-fold enhancement), a number of heavy fermion materials display highly unusual superconductivity (HFSCs) [1]. Indeed, the heavy electrons themselves pair (as evidenced by the scaling of the specific heat jump at the transition temperature T_c with the normal state specific heat). Unconventional superconducting order parameters (pair wave functions) with either spatial [2] or temporal nodes (so called "odd-frequency" pairing) [3–7] avoid the strong Coulomb interaction and so are favored for interpreting these systems. This view is supported by observation of (i) power laws in low temperature physical properties [1,2], in contrast with the activated behavior of conventional (nodeless) pair wave functions of, e.g., aluminum, and (ii) the complex multiphase superconductivity of UPt_3 and $U_{1-x}Th_xBe_{13}$ (and possibly UBe_{13} itself) [1,2,8]. The superconductivity coexists with antiferromagnetism (AFM) (AFM-usually commensurate) in UPt_3, URu_2Si_2, UPd_2Al_3, and UNi_2Al_3 [1], and competes with AFM in $CeCu_2Si_2$ [9]. Finally, at least in UBe_{13} [10] and $CeCu_2Si_2$ [9], the "normal metallic state" is clearly *not* described as a Fermi liquid. In each of these materials above T_c, the linear specific heat rises with decreasing temperature, the resistivity is approximately linear in T, and the residual resistivity at T_c is high (typically 80–100 $\mu\Omega$ cm in the best samples of UBe_{13}).

In this paper, we provide the first calculations of the phase diagram for the two-channel Kondo lattice in infinite spatial dimensions. We find second order antiferromagnetic and first order odd-frequency superconducting phase transitions. Coexistence of commensurate (and incommensurate) antiferromagnetism with superconductivity is, in principle, possible. We present several possible routes to account for the multiple superconducting phases observed in real materials. Taken together with the non-Fermi liquid paramagnetic phase discussed in previous publications [11], and earlier suggestions that the two-channel lattice may describe UBe_{13} and other heavy fermion systems [8], our work establishes that the two-channel Kondo lattice model possesses the key ingredients needed to explain HFSC.

Motivation.—A possible model for some heavy fermion compounds is the two-channel Kondo lattice which consists of two identical species of noninteracting electrons antiferromagnetically coupled to a lattice of spin $1/2$ Kondo moments [8]. This model displays non-Fermi liquid behavior because of the overcompensation of the Kondo spins by the conduction electrons. This was first pointed out in the single site two-channel model by Nozières and Blandin [12]; the impurity plus extended conduction screening clouds yield a net spin $1/2$ character. This yields a degenerate ground state with a non-Fermi liquid excitation spectrum. This overscreening also effects an interchannel pairing mechanism [8], which in the impurity problem favors spin-singlet channel-singlet odd-frequency superconducting fluctuations [5–7]. We find that this overscreening generates novel antiferromagnetic superexchange between the Kondo spins on the lattice. Taken together with the RKKY exchange, this favors antiferromagnetism in the lattice model close to half-filling of the two channels. In this paper we will elucidate the nature of the superconducting and magnetic transitions on the lattice.

Model.—The Hamiltonian for the two-channel Kondo lattice is

$$H = J\sum_{i,\alpha}\mathbf{S}_i \cdot \mathbf{s}_{i,\alpha} - \frac{t^*}{2\sqrt{d}}\sum_{\langle ij\rangle,\alpha,\sigma}(c^{\dagger}_{i,\alpha,\sigma}c_{j,\alpha,\sigma} + \text{H.c.}) - \mu\sum_{i,\alpha,\sigma}c^{\dagger}_{i,\alpha,\sigma}c_{i,\alpha,\sigma}\,, \qquad (1)$$

where $c^{\dagger}_{i,\alpha,\sigma}$ ($c_{i,\alpha,\sigma}$) creates (destroys) an electron on site i in channel $\alpha = 1, 2$ of spin σ, $\mathbf{S}_i$ is the Kondo spin on site i, and $\mathbf{s}_{i,\alpha}$ are the conduction electron spin operators for site i and channel α. The sites i form an infinite-dimensional hypercubic lattice. Hopping is limited to nearest neighbors with hopping integral $t \equiv t^*/2\sqrt{d}$. All energies are measured in units of the scaled hopping integral t^*. Thus, on each site the Kondo spin mediates an interaction between the two different channels. This problem is nontrivial, and for the region of interest in which $J > 0$ and $T \ll J, t^*$ it is describable only with nonperturbative approaches.

 0031-9007/97/78(10)/1996(4)$10.00

Formalism and Simulation.—Metzner and Vollhardt [13] provided a simplified method for solving such problems in a nontrivial limit. They observed that the renormalizations due to local two-particle interactions become purely local for the coordination number tending to infinity. In consequence, most standard lattice models may be mapped onto the solution of an effective correlated impurity coupled to a self-consistently determined bath or medium (see [14] for further details and references).

We solve the effective impurity problem for Eq. (1) by using the quantum Monte Carlo (QMC) algorithm of Fye and Hirsch [15], modified for the two-channel Kondo model [16]. We simulated the model for several fillings N $(0 < N \leq 1)$ and exchange interaction strengths J ($J = 0.75,\ 0.625,\ 0.5,\ 0.4$). Error bars on the measured quantities are less than 6% for the results presented here. A sign problem encountered in the QMC process prevented us from studying $J \gtrsim 0.8$ and $N \lesssim 0.5$ since lower temperatures are required to access the physically interesting regime.

The QMC simulation naturally produces both one- and two-particle properties. The local spin susceptibility χ_L was obtained by measuring the three-by-three matrix of the local susceptibility, including both the Kondo spin and conduction band spin fluctuations. χ was then inverted to calculate the associated irreducible vertex function and the corresponding lattice susceptibility in the usual way [17].

The situation for the superconductivity is more complicated. Only the two conduction channels contribute to the pair-field susceptibility. We can then look for pairing instabilities in singlet and triplet channels for both spin and channel. Motivated by impurity model results [5,6], we have restricted our attention to the particle-particle propagator diagrams as shown in Fig. 1. It is possible to make two independent combinations of these diagrams, viz., $\chi_{\pm}(i\omega_n, i\omega_m, \vec{q}) = \chi_{11}(i\omega_n, i\omega_m, \vec{q}) \pm \chi_{12}(i\omega_n, i\omega_m, \vec{q})$, from which we construct a quartet of spin and channel, singlet and triplet pair-field susceptibilities given by

$$P_{\mathrm{SsCs}}(\vec{q},T) = T\sum_{nm} f_-(i\omega_n)\chi_-(i\omega_n, i\omega_m, \vec{q}) f_-(i\omega_m)\,, \tag{2}$$

$$P_{\mathrm{StCt}}(\vec{q},T) = T\sum_{nm} f_+(i\omega_n)\chi_+(i\omega_n, i\omega_m, \vec{q}) f_+(i\omega_m)\,, \tag{3}$$

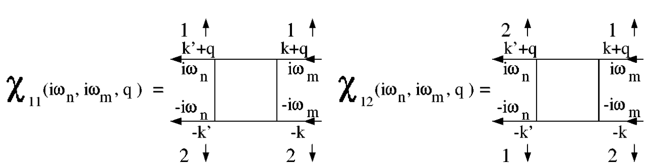

FIG. 1. Particle-particle interchannel opposite spin diagrams which contribute to the pair-field susceptibility. Here 1 and 2 label the channel, and ↑ and ↓ the spin. Summing over $\vec{k}$ and $\vec{k}'$ yields χ_{11} and χ_{12}.

$$P_{\mathrm{StCs}}(\vec{q},T) = T\sum_{nm} \chi_-(i\omega_n, i\omega_m, \vec{q})\,, \tag{4}$$

$$P_{\mathrm{SsCt}}(\vec{q},T) = T\sum_{nm} \chi_+(i\omega_n, i\omega_m, \vec{q})\,. \tag{5}$$

Here $f_{\pm}(i\omega_n)$ are odd functions of Matsubara frequency used to project out the odd-frequency pairing, and, for example, $P_{\mathrm{SsCs}}(\vec{q},T)$ is the spin-singlet channel-singlet pair-field susceptibility for a pair with center-of-mass momentum $\vec{q}$.

To determine the form of $f_{\pm}(i\omega_n)$, we have employed the pairing matrix formalism of Owen and Scalapino [18]. We have represented each $\chi_{\pm}$ in a two-particle Dyson equation and extracted the irreducible vertex functions $\Gamma_{\pm}$. The resulting pairing matrices are

$$M_{\pm}(i\omega_n, i\omega_m, \vec{q}) = \sqrt{\chi^0_{\pm}(i\omega_n, \vec{q})}\,\Gamma_{\pm}(i\omega_n, i\omega_m) \times \sqrt{\chi^0_{\pm}(i\omega_m, \vec{q})}\,, \tag{6}$$

where $\chi^0_{\pm}(i\omega_n, \vec{q})$ are the particle-particle diagrams in Fig. 1 without vertex corrections. $f_{\pm}(i\omega_n)$ is the eigenvector corresponding to the dominant eigenvalue of $M_{\pm}$ (that with the largest absolute value).

Results.—In this model, antiferromagnetism is driven by both RKKY interactions and a novel type of superexchange. The latter arises from hopping between adjacent spin $1/2$ screening clouds, whose overall spin is determined by the conduction electrons; the Pauli principle forbids hopping unless neighboring spins in the same channel are antiparallel. As a result, for large J, the superexchange goes as $\sim(t^*)^2/J$. For conduction band fillings close to $N = 1$, both the RKKY (evaluated at nearest neighbor sites) and the superexchange favor antiferromagnetism (the RKKY exchange remains antiferromagnetic until $N \lesssim 0.5$), and an antiferromagnetic transition results, as shown in Fig. 2. Because of the screening of the local moments by the conduction spin, the transition is very weak, as measured by the full susceptibility. Specifically, χ_{AF} is not significantly enhanced over the bulk susceptibility χ_F until $T \gtrsim T_N$. However, the f-electron contribution to the susceptibility shows a protracted scaling region. Note that screening affects nonlinear feedback which reduces the susceptibility exponent γ from the mean-field value $\gamma = 1$. γ increases with doping ($N < 1$), and the transition becomes incommensurate as $T_N \to 0$.

To explore superconductivity, it is necessary to find the frequency form factors $f_{\pm}$ discussed previously. As the temperature is lowered, the dominant eigenvalue first becomes large (divergent) and negative, and then abruptly switches to a large and positive value at the transition. This happens first in M_-, and the corresponding eigenvector of M_- is plotted in the inset to Fig. 3. It can be fit quite accurately to the form $T/2\omega_n$ as shown by the solid line, which corresponds to the form factor of Ref. [4]. Thus, we use $f_-(i\omega_n) = T/2\omega_n$ to project out the odd-frequency pair-field susceptibilities shown in

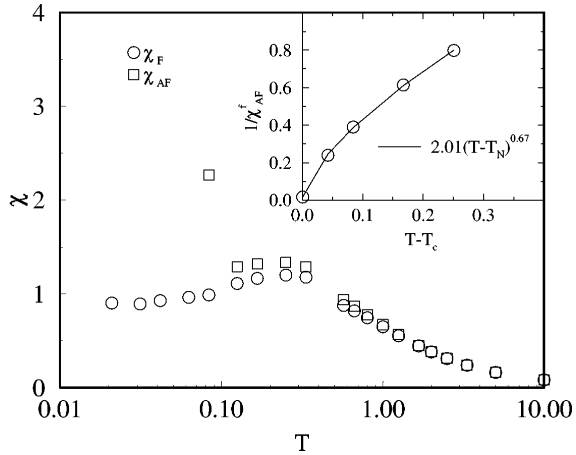

FIG. 2. Antiferromagnetic χ_{AF} and ferromagnetic χ_F susceptibilities of the two-channel Kondo lattice with $J = 0.75$ and $N = 1.0$. Inset: the local moment contribution to the susceptibility $\chi^f_{AF}(T)$, which displays a protracted scaling region well fit by $1/\chi^f_{AF}(T) \simeq a(T - T_N)^\gamma$. Strong conduction screening of local moments is indicated by (i) $\chi_{AF} \neq \chi^f_{AF}(T)$ and (ii) $\gamma < 1$.

Figs. 3 and 4. [Other form factors $f(i\omega_n) = \tanh(T_0/\omega_n)$ and $\mathrm{sgn}(\omega_n)$ produce qualitatively similar results.]

The first transition is found in the spin-singlet channel-singlet pairing combination, as shown in Fig. 3. (Note that this pair state is even in parity, so that the odd-frequency condition enforces the Pauli principle, in contrast with the odd-parity and odd-frequency spin-singlet pairs of the single-channel case [3,4].) To interpret this result, remember that the inverse pair-field susceptibility is proportional to the curvature of the free energy $f(\Delta_{\mathrm{SsCs}})$ as a function of the pairing order parameter $1/P_{\mathrm{SsCs}} \propto d^2f(\Delta_{\mathrm{SsCs}})/d\Delta^2_{\mathrm{SsCs}}$. Thus, if $P_{\mathrm{SsCs}} < 0$ a thermodynamic instability of the system is present. The associated transition cannot be continuous, since this requires the free energy in order parameter space to become flat (i.e., P_{SsCs} diverges) so that the order parameter may change continuously. Thus, we identify this as a discontinuous transition. Furthermore, if $P_{\mathrm{SsCs}}(T^*) = 0$, then T^* is a lower bound to the transition temperature since, when $P_{\mathrm{SsCs}}(T - T^* = 0^-) = 0^-$, the curvature of $f(\Delta_{\mathrm{SsCs}})$ is divergent and negative; i.e., the free energy displays a downward cusp which would compel the order parameter and the free energy to change discontinuously at T^*, which involves an infinite energy at the transition. Hence, the actual transition occurs at a temperature $T_c > T^*$.

Several remarks are in order about this unusual superconductivity: (a) Figure 3 suggests that the transition is degenerate at the zone center and the zone corner, and, in fact, P_{SsCs} vanishes simultaneously over the whole zone, and hence this is a *locally* driven transition. This degeneracy will be lifted in finite dimensionality as the superfluid stiffness Υ_s (analogous to spin stiffness in a magnet) must vanish in infinite d. For finite d with $\Upsilon_s(\vec{q} = 0) > 0$ (< 0), a local free energy minimum will be found at $\vec{q} = 0$ ($\vec{q} \neq 0$). (b) The vanishing of the local pair susceptibility here at T^* contrasts with the impurity model in which it diverges logarithmically as $T \to 0$ [5,6]. (c) The excitation spectrum of such a transition may well be highly exotic [4].

As shown in Fig. 4, the ground state of the system may be superconducting or magnetic, which may coexist or compete. Detailed exploration within the ordered phases will answer this question definitively, as the present work only indicates the presence of transitions. In general superconductivity will occur first (at the highest transition temperature) away from half-filling, and antiferromagnetism will occur first near half-filling. However, for values of $J > 0.75$, we found that superconductivity occurs

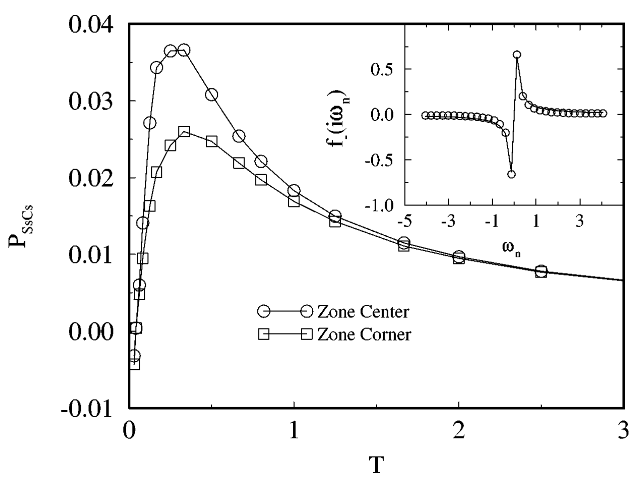

FIG. 3. Odd-frequency (spin-singlet, channel-singlet) pair-field susceptibility. At $T = T^* = 0.041 \leq T_c$, $P_{\mathrm{SsCs}}(T)$ becomes negative for both zone-center and zone-corner pairs, indicating a discontinuous transition to a paired state. Inset: the dominant zone-center eigenvector [or form factor f_- of Eqs. (2)–(5)] of the pairing matrix M_- vs Matsubara frequency; $f_- \simeq 0.5T/\omega_n$ as in Ref. [4].

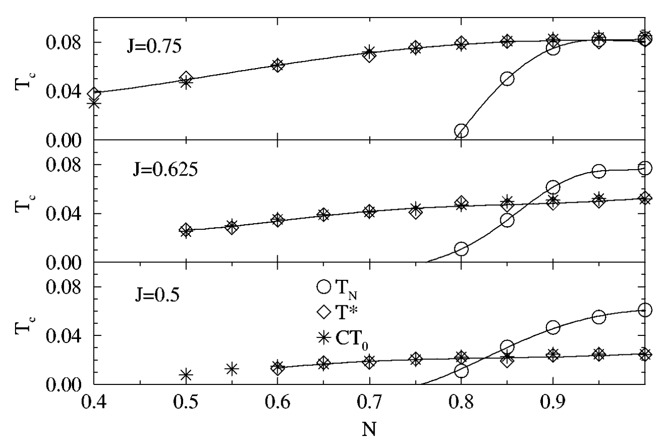

FIG. 4. Phase diagrams of the two-channel Kondo lattice for various values of J. The solid lines are fits to the data. The antiferromagnetic transition becomes incommensurate near $T_N \to 0$. The temperature $T^* \approx CT_0$ is a lower bound to the first order superconducting transition temperature (cf., Fig. 3); here $C = 0.43(J = 0.5)$, $0.51(J = 0.625)$, $0.58(J = 0.75)$.

first even at half-filling (the minus sign problem precluded a systematic study for these values of J so they are not presented in Fig. 4). We also found that $T^* \approx C(J)T_0$, with $C(J) \approx 0.5$ and weakly dependent on J. In contrast, T_N appears to depend upon both J and T_0.

Speculation and Interpretation.—We offer two compatible interpretations of the result $T^* \approx 0.5T_0$. First, T_0 is the local dynamic energy scale, and thus this result underscores the local origin of the pairing. Second, $T \approx 0.5T_0$ is also the temperature at which the slope of the real part of the self-energy becomes one [11], so that the quasiparticle renormalization factor diverges. This result suggests that, when the system cannot form a Fermi liquid due to a large residual scattering rate (with concomitant residual entropy), it forms a superconducting state to quench the entropy. The antiferromagnetic transition temperature, on the other hand, depends upon both J (through the intersite exchange) and T_0 (through moment screening and superexchange). As noted above, we cannot determine whether these states coexist without a detailed exploration within the ordered phases. At half-filling, where the antiferromagnetism produces an insulating phase, clearly the superconductivity will be suppressed for $J \leq 0.75$.

Our results offer a number of routes to be explored for explaining the complex superconducting phase diagrams of UPt_3 and $U_{1-x}Th_xBe_{13}$: (1) *Competition between phases with a multipoint irreducible star:* As mentioned above, for $\Upsilon_s < 0$ in finite d, $\vec{q} \neq 0$ pairs are favored, quite likely at the Brillouin zone corner for such a bipartite lattice. For lattices with frustration, such as hexagonal UPt_3 and fcc UBe_{13}, multipoint irreducible stars may be needed to describe staggered order parameters which can then have multiple phases [19]. (2) *Competition between different $\vec{q}$ values:* As noted above, T^*, the lower bound for the first order superconducting transition temperature, is independent of $\vec{q}$ in our calculations. Thus multiple phases may thus correspond to superconducting transitions with different $\vec{q}$ values. (3) *Possible instability of spin-triplet/channel-triplet pairing:* At yet lower temperatures than those identified in Fig. 4, we observe a sign change in the pair-field susceptibility associated with spin triplet-channel triplet odd-frequency pairing. Hence it is possible that the competition between this triplet-triplet and the singlet-singlet odd-frequency pairing may explain the complex phase diagrams.

In conclusion, we note that this superconducting transition can agree with experiment only if it is weakly first order; this is plausible given the rapid change in free energy curvature at the order parameter origin. Detailed investigations in the ordered phase will resolve this issue, and whether any of the above scenarios can describe the complex phase diagrams of UPt_3 and $U_{1-x}Th_xBe_{13}$.

We would like to acknowledge useful discussions with F. Anders, A. V. Balatsky, W. Chung, A. Georges, B. Goodman, D. Hess, H. R. Krishna-murthy, M. Ma, A. J. Millis, and W. Putikka. M. J. and H. P. would like to acknowledge the support of NSF Grants No. DMR-9406678 and No. DMR-9357199. D. L. C. acknowledges the support of the NSF under Grant No. DMR-9420920. Computer support was provided by the Ohio Supercomputer Center.

[1] Some good recent reviews are the following: N. Grewe and F. Steglich, *Handbook on the Physics and Chemistry of Rare Earths,* edited by K. A. Gschneidner, Jr., and L. L. Eyring (Elsevier, Amsterdam, 1991), Vol. 14, p. 343; D. W. Hess, P. S. Riseborough, and J. L. Smith, *Encyclopedia of Applied Physics,* edited by G. L. Trigg (VCH Publishers Inc., New York, 1993), Vol. 7, p. 435; H. R. Ott, J. Low Temp. Phys. **95**, 95 (1994).
[2] J. A. Sauls, Adv. Phys. **43**, 113–141 (1994).
[3] V. L. Berezinski, JETP Lett. **20**, 287 (1974); A. V. Balatsky and E. Abrahams, Phys. Rev. B **45**, 13 125 (1992); E. Abrahams *et al.*, Phys. Rev. B **52**, 1271 (1995).
[4] P. Coleman, E. Miranda, and A. Tsvelik, Phys. Rev. Lett. **70**, 2960 (1993); P. Coleman, E. Miranda, and A. M. Tsvelik, Phys. Rev. B **49**, 8955 (1994).
[5] V. J. Emery and S. Kivelson, Phys. Rev. B **46**, 10 812 (1992).
[6] A. W. W. Ludwig and I. Affleck, Nucl. Phys. **B428**, 545 (1994).
[7] Enhanced staggered odd-frequency pairing correlations exist in the one-dimensional Kondo lattice when left and right movers approximately decouple, rendering effectively a two-channel lattice; see O. Zachar, S. Kivelson, and V. Emery, Phys. Rev. Lett. **77**, 1342 (1996).
[8] D. L. Cox, Phys. Rev. Lett. **59**, 1240 (1987); D. L. Cox, Physica (Amsterdam) **153C-155C**, 1642 (1988); D. L. Cox, Physica (Amsterdam) **186B-188B**, 312 (1993); D. L. Cox and M. B. Maple, Phys. Today **48**, 32 (1995); D. L. Cox and M. Jarrell (unpublished).
[9] F. Steglich *et al.*, Physica (Amsterdam) **223B-224B**, 1 (1996).
[10] This was noted much earlier in H. R. Ott, Prog. Low Temp. Phys. **6**, 215 (1987).
[11] M. Jarrell, H.-B. Pang, D. L. Cox, and K.-H. Luk, Phys. Rev. Lett. **77**, 1612 (1996); M. Jarrell, H.-B. Pang, and D. L. Cox (unpublished); F. Anders, M. Jarrell, and D. L. Cox (unpublished).
[12] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).
[13] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); see also E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989).
[14] Th. Pruschke, M. Jarrell, and J. K. Freericks, Adv. Phys. **42**, 187 (1995); A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[15] R. M. Fye and J. E. Hirsch, Phys. Rev. B **38**, 433 (1988).
[16] K.-H. Luk, Mark Jarrell, and D. L. Cox, Phys. Rev. B **50**, 15 864 (1994).
[17] M. Jarrell, Phys. Rev. B **51**, 7429 (1995).
[18] C. Owen and D. J. Scalapino, Physica (Amsterdam) **55**, 691 (1971).
[19] R. Heid, Ya. B. Bazaliy, V. Martisovits, and D. L. Cox, Phys. Rev. Lett. **74**, 2571 (1995).