One-Dimensional Kondo Lattice at Partial Band Filling

Graeme Honner and Miklós Gulácsi
Department of Theoretical Physics, Institute of Advanced Studies, The Australian National University, Canberra, ACT 0200, Australia
(Received 8 July 1996)

An effective Hamiltonian for the localized spins in the one-dimensional Kondo lattice model is derived via a unitary transformation involving a bosonization of *delocalized* conduction electrons. The effective Hamiltonian is shown to reproduce all the features of the model as identified in various numerical simulations, and provides much new information on the ferromagnetic to paramagnetic phase transition and the paramagnetic phase. [S0031-9007(97)02679-3]

PACS numbers: 71.27.+a, 71.28.+d, 75.20.Hr

The Kondo lattice model (KLM) describes the interaction between a conduction band and a half-filled narrow f band, and is thought to capture the essential physics of some of the rare-earth compounds [1]. Although intensively studied for two decades, the KLM is still far from being completely understood. Even in the simple one-dimensional (1D) model, and with the conduction band less than half filled, there are only two limits in which the behavior has been analyzed successfully; in the limit of vanishing conduction electron (CE) density, and for antiferromagnetic Kondo couplings $J > 0$, the f electrons (f spins) form a ferromagnetic (FM) ground state [2]; in the strong-coupling limit $J \to \infty$, and for any filling of the conduction band, the unpaired f spins are again found to be FM [3]. The intermediate to weak coupling regime, away from half filling but at finite CE density, has proved particularly difficult to analyze [3].

From the known limiting behavior [2,3], together with a consensus of recent numerical simulations using the density-matrix renormalization group, exact numerical diagonalization, and quantum Monte Carlo [4–6], a successful theory of the less than half-filled 1D KLM will account for the following ground-state behavior of the f spins: (i) At strong to intermediate coupling the unpaired f spins are FM at all fillings and show behavior in accord with the strong-coupling expansion [3]. (ii) As the coupling is lowered, and for finite CE density, the system undergoes a transition to a paramagnetic (PM) state, with a filling dependent critical coupling in the weak to intermediate range. (iii) At weak coupling, the system is characterized by a strong peak in the f-spin structure factor at $2k_F$ of the CEs.

In this Letter we derive an effective Hamiltonian H_{eff} from the 1D KLM which reproduces *all* the observed behavior in the intermediate to weak coupling regime. H_{eff} treats the f spins exactly while the CEs are treated using bosonization techniques. The essential new ingredient in our work is an emphasis on describing delocalized CEs, as these are responsible for the observed magnetic behavior of the f spins. The problem of accessing the intermediate to weak coupling regime nonperturbatively is solved using a unitary transformation. The effective Hamiltonian maps to the quantum random transverse-field Ising spin chain near the FM-PM boundary, and using extensive work on this interesting model by Fisher [7], we can obtain a vast amount of information on the transition and the properties of the model near it, as well as information on the PM phase.

The Hamiltonian of the 1D KLM is given by

$$H = -t \sum_{j\sigma} (c^{\dagger}_{j\sigma} c_{j+1\sigma} + \text{ H.c.}) + J \sum_{j} \mathbf{S}_{fj} \cdot \mathbf{S}_{cj}\,, \quad (1)$$

where $t > 0$ is the CE hopping, $\mathbf{S}_{fj} = \frac{1}{2} \sum_{\sigma,\sigma'} c^{\dagger}_{fj\sigma} \times \boldsymbol{\sigma}_{\sigma,\sigma'} c_{fj\sigma'}$, $\mathbf{S}_{cj} = \frac{1}{2} \sum_{\sigma,\sigma'} c^{\dagger}_{j\sigma} \boldsymbol{\sigma}_{\sigma,\sigma'} c_{j\sigma'}$, and $\boldsymbol{\sigma}$ are the Pauli spin matrices. Fermi operators $c_{j\sigma}, c^{\dagger}_{j\sigma}$ with subscript f refer to localized f spins, those without refer to the CEs. We consider antiferromagnetic Kondo couplings $J > 0$ and assume the conduction band filling $n = N_c/2N < \frac{1}{2}$ with N_c the number of CEs and N the number of sites.

From the strong-coupling expansion [3], it is clear that the infinite J on-site spin singlets, in which a CE is strictly localized with an f spin, are magnetically inert: The strong-coupling FM appears only at large but finite J via CE hopping to neighboring unpaired sites, with a preferred spin orientation due to broken spin-singlet symmetry. The interaction identified in the strong-coupling expansion is the Zener double-exchange mechanism. This motivates us to introduce a *delocalization length* $\alpha > a$ (a the lattice spacing) which limits the minimum spatial spread of the CEs. The delocalization length models the qualitative difference between large J and infinite J behaviors, and has its physical basis in the energy gain for CE hopping to unpaired f spins whenever $t > 0$. It relates to the average spatial spread of the CEs engaged in the double exchange process. For example, the delocalization length in the one CE KLM corresponds to the effective spread of the spin polaron [2]. For simplicity, α will be taken as an average applying uniformly to the CEs. It is important to emphasize that α limits only the *minimum* spread of the CEs and does not significantly affect the weak coupling behavior, although it is essential in order to describe the strong-coupling FM.

 0031-9007/97/78(11)/2180(4)$10.00

It is well known that 1D electrons may be represented using bosonization techniques. The Bose description is usually based on the Luttinger model due to its formal rigor, but this is not essential. In the present case it is essential *not* to use the Luttinger model, as will become clear. Two facts, peculiar to 1D, form the basis of bosonization for realistic 1D systems. The first is Tomonaga's observation [8] that the number fluctuation operators satisfy Bose-like commutation relations $[\rho_{r\sigma}(k), \rho_{r'\sigma'}(k')] = \delta_{r,r'}\delta_{k,-k'}\delta_{\sigma,\sigma'} rkL/2\pi$ on a weak coupling long-wavelength subspace, where the right-moving ($r = +$) and left-moving ($r = -$) number fluctuations

$$\rho_{r\sigma}(k) = \sum_{0<rp<\pi/a} c^{\dagger}_{p-\frac{k}{2}\sigma} c_{p+\frac{k}{2}\sigma}$$

with $L = Na$. The second is the fact that these number fluctuations generate the 1D state space [9]. The main result from bosonization needed here is the representation of the Fermi site operators $c_{j\sigma}$ in terms of the bosonic number fluctuations $\rho_{r\sigma}(k)$. It is convenient to decompose the site operators into right- and left-moving components $c_{j\sigma} = \sum_r c_{rj\sigma}$:

$$c_{rj\sigma} = \frac{1}{\sqrt{N}} \sum_{k_F-\frac{1}{2\alpha}<rk<k_F+\frac{1}{2\alpha}} e^{ikja}\, c_{k\sigma}\,,$$

with $k_F = \pi n/a$, and where the momentum cutoff comes from Fourier analysis. In the Luttinger model the Bose representation may be formulated as an operator identity [10]. For the realistic system we must be satisfied with an approximate representation, but one which generates asymptotically exact results [11]. (The *existence* of the representation is guaranteed by the completeness of the Bose states.) In the thermodynamic limit,

$$c_{rj\sigma} \approx \mathcal{N}(\alpha) e^{irk_F ja}\, e^{i\{\theta_\rho(j)+r\phi_\rho(j)+\sigma[\theta_\sigma(j)+r\phi_\sigma(j)]\}/2}, \quad (2)$$

where the Bose fields for $\nu = \rho, \sigma$ are defined by $\psi_\nu(j) = i(\pi/L)\sum_{k\neq 0} e^{ikja}[\nu_+(k) \pm \nu_-(k)]\Lambda(k)/k$, with $+$ corresponding to the number fields $\psi_\nu = \phi_\nu$ and $-$ to the current fields $\psi_\nu = \theta_\nu$. The charge and spin number fluctuations $\rho_r(k) = \sum_\sigma \rho_{r\sigma}(k)$, and $\sigma_r(k) = \sum_\sigma \sigma\rho_{r\sigma}(k)$. Equation (2) has the same form as in the Luttinger model but with one crucial difference. The even cut-off function $\Lambda(k)$, satisfying $\Lambda(k) \approx 1$ for $|k| < 1/\alpha$ and $\Lambda(k) \approx 0$ otherwise, is needed in the Bose fields to ensure that delocalized CEs are described. The normalization factor $\mathcal{N}(\alpha)$ depends on both the cutoff and the cutoff function, and can be determined only asymptotically. Equation (2) will, of course, fail if it is used to calculate number operators $n_{rj\sigma} = c^{\dagger}_{rj\sigma} c_{rj\sigma}$. In this case a Fourier expansion gives

$$n_{rj\sigma} = -\frac{a}{4\pi}\partial_x\{\phi_\rho(j) + r\theta_\rho(j) + \sigma[\phi_\sigma(j) + r\theta_\sigma(j)]\} \quad (3)$$

to an additive constant. The separate form for the number operators is manifest also in the Luttinger model and is accounted for there with a carefully constructed normal ordering convention and a prescription for the correct taking of limits [10].

To derive an effective interaction between the f spins from the bosonized Hamiltonian [obtained by substituting Eqs. (2) and (3) into Eq. (1)], it is sufficient to change to a basis of states in which the CEs are coupled to the f spins. This is achieved using a unitary transformation with $U = i(aJ/2\pi v_F)\sum_j S^z_{fj}\theta_\sigma(j)$, and where $v_F = 2at\sin(\pi n)$. A variant of this transformation was first used by Emery and Kivelson for the single-impurity Kondo problem, and later generalized to the 1D KLM [12]. The usage here is different; indeed the FM J^2 term [see Eq. (4) below], which U was designed to generate, is entirely absent in the previous work. The reason is that a Luttinger model bosonization will miss any f-spin effective interaction which is due to the *nonlocal* character of the CEs. Formally, in the Luttinger model the Bose fields $\phi_\nu(j)$ and $\Pi_\nu(j) = -\partial_x\theta_\nu(j)$ are canonically conjugate and their commutator strictly vanishes unless they are at the same site. In our system the fields are smeared over a range α and their commutator is finite over roughly $2\pi\alpha$: $[\phi_\nu(j), \Pi_{\nu'}(0)] = 2i\delta_{\nu,\nu'}J_j(\alpha)$, where $J_j(\alpha) = \int_0^\infty \cos(kja)\Lambda^2(k)dk$. As examples, a Gaussian $\Lambda(k) = \exp(-\alpha^2k^2/2)$ gives $J_j(\alpha) = (\sqrt{\pi}/2\alpha)\exp[-(ja/2\alpha)^2]$, and the Luttinger cutoff $\exp(-\alpha|k|/2)$ gives $J_j(\alpha) = \alpha/[\alpha^2 + (ja)^2]$. The Luttinger model δ function is obtained by taking $\alpha \to 0$ in the last. The effect of this difference on the transformed Hamiltonian $\tilde{H} = e^{-U}He^{U}$ is dramatic. Keeping all terms,

$$\tilde{H} = \frac{av_F}{4\pi}\sum_{j,\nu}\{\Pi^2_\nu(j) + [\partial_x\phi_\nu(j)]^2\} - \frac{a^2J^2}{4\pi^2v_F}\sum_{j,j'} J_{j-j'}(\alpha) S^z_{fj}S^z_{fj'} + J\mathcal{N}^2(\alpha)\sum_j [e^{i(1-\frac{aJ}{2\pi v_F})\theta_\sigma(j)} S^+_{fj} + \text{H.c.}]$$
$$\times \{\cos[K(j) - \phi_\sigma(j)] + \cos[2k_Fja + \phi_\rho(j)]\} + 2J\mathcal{N}^2(\alpha)\sum_j \sin[K(j) - \phi_\sigma(j)]\sin[2k_Fja + \phi_\rho(j)]S^z_{fj}\,, \quad (4)$$

where $K(j) = -i(aJ/2\pi v_F)\sum_{j'}[\phi_\nu(j), \theta_\nu(j')]S^z_{fj'}$. A condition for the derivation of Eq. (4) is that the cutoff be not too soft.

The new term in Eq. (4) is the second. Since S^z_{fj} is not transformed under U, it is immediate that the system is FM at intermediate coupling at all fillings. The physical basis for the interaction is quite simple. A CE spread over more than one lattice site will carry the same spin over these sites. Because of the term $J\sum_j(n_{rj\uparrow} - n_{rj\downarrow})S^z_{fj}$ in Eq. (1), this will tend to align

the relevant f spins. This interpretation also makes it clear that the interaction $J_j(\alpha)$ is short range provided α is finite. We may therefore approximate the FM term by its nearest-neighbor form $-J_{\rm eff}\sum_j S^z_{fj}S^z_{fj+1}$, $J_{\rm eff} = (a^2J^2/2\pi^2 v_F)J_1(\alpha)$. Although formally this term will give FM at strong coupling as well, it is important to recall that the bosonization describes delocalized CEs. If J is too large then there will be significant CE localization and our approximation is less satisfactory. Note that it is in principle possible to include these effects as well with a less crude measure of CE delocalization and with the sum over j in the FM term restricted to sites containing unpaired f spins only. Such alterations will not affect our conclusions, except to further support them.

An effective Hamiltonian for the f spins is obtained from Eq. (4) by replacing the CE Bose fields by their expectation values in the noninteracting ground-state. This step may be justified for the Bose charge-number field $\phi_\rho(j)$ by noting that at weak coupling, which is the only regime where any of the fields affect Eq. (4), the charge structure factor is free electron like [6]. For the spin fields there is less justification, though note that at weak coupling these fields will be relatively smooth and will enter Eq. (4) as simple parameters. Thus while this approximation may affect the quantitative predictions of the theory, it would not be expected to affect the qualitative behavior. (Further evidence for this view was recently provided in a numerical simulation in which the same general behavior for the f spins was seen with t-J interacting CEs [13].) The effective Hamiltonian is then

$$-H_{\rm eff} = J_{\rm eff}\sum_j S^z_{fj}S^z_{fj+1} + 2J\mathcal{N}^2(\alpha)\sum_j[\cos K(j) + \cos(2k_F ja)]S^x_{fj} + 2J\mathcal{N}^2(\alpha)\sum_j \sin K(j)\sin(2k_F ja)S^z_{fj}, \quad (5)$$

and the spin directions have been reversed for later convenience. Equation (5) is our main result. The remainder of this Letter is concerned with a brief analysis of $H_{\rm eff}$ to show that it gives all the required behavior. Details will be presented in a paper to follow [14].

To describe the destruction of the FM phase, the $S^z_{fj'}$ in $K(j)$ may be replaced by their eigenvalues. $K(j)$ is then a long-range object which counts the total S^z_f to the left of j and subtracts from that the total S^z_f to the right. **(**The effects of the non-Luttinger bosonization are not important here; $[\phi_\nu(j'),\theta_\nu(0)] \to i\pi\ \mathrm{sgn}(j')$ at large j'.**)** Near the FM phase boundary, and in the thermodynamic limit, it follows that $K(j) \approx 0$ and any transition is described by the first two terms in $H_{\rm eff}$, with the second term responsible for spin flips. For incommensurate fillings, $\cos(2k_F ja)$ oscillates unsystematically with respect to the lattice. The large values $\cos(2k_F ja) \approx 1$, which are responsible for spin flips, are then widely separated. Following analogous treatments in spin glasses [15], this behavior is well described by taking $\cos(2k_F ja)$ as a random variable. The factor multiplying S^x_{fj} in Eq. (5) is then replaced by h_j, where h_j is drawn independently from the displaced cosine distribution $\rho(h)dh$ where $\rho(h) = (1/C\pi)\{1 - [(h/C) - 1]^2\}^{-1/2}$ and $C = 2J\mathcal{N}^2(\alpha)$. Note that fluctuations in the Bose charge-number fields $\phi_\rho(j)$ offer further support for this interpretation. The behavior of the f spins at and near the destruction of the FM phase is then governed by the quantum random transverse-field Ising spin Hamiltonian $H_{\rm crit} = -J_{\rm eff}\sum_j S^z_{fj}S^z_{fj+1} - \sum_j h_j S^x_{fj}$. Using extensive real space renormalization-group work on this model by Fisher [7] (to whom we refer the reader for details), we determine the location of the quantum critical line describing the order-disorder transition at

$$\frac{J}{t} = \frac{4\pi^2\mathcal{N}^2(\alpha)}{aJ_1(\alpha)}\sin(\pi n). \quad (6)$$

The numerical predictive powers of $H_{\rm eff}$ are restricted by lack of knowledge of $\mathcal{N}(\alpha)$. We would like to emphasize that such problems beset *any* bosonization description in which physical quantities are found to depend on this factor, and are not due to our particular bosonization. Accordingly, the coefficient of $\sin(\pi n)$ in Eq. (6) is used as a fitting parameter to numerically obtained critical points [4–6]. A good fit is obtained with $J/t = 2.5\sin(\pi n)$, as shown in Fig. 1. Note that this ignores any functional dependence of α on J or n.

For the following discussion, it is convenient to introduce a measure of deviation from criticality $\delta \propto \ln[2\pi^2\mathcal{N}^2(\alpha)v_F/a^2JJ_1(\alpha)]$ [7], which for the obtained fit is $\delta \propto \ln[2.5t\sin(\pi n)/J]$.

The behavior described by $H_{\rm crit}$ is simply understood in terms of *clusters* of ordered f spins. Reducing J from intermediate values in the FM phase, the infinite cluster characterizing strong FM is broken up into several large clusters as the quantum fluctuations h_j, controlled by the spin-flip interactions, become stronger. The individual clusters are the spin polarons. The system is weakly ordered and exists for $-0.7 < \delta < 0$ with the boundary determined by $J_{\rm eff} = \max\{h_j\}$, as shown in Fig. 1. This is not a true transition line, but rather marks the onset of a Griffiths phase [16] characterized by singularities in the free energy over the whole range of δ. For small δ the correlation length is $\xi \sim \delta^{-2}$, beyond which the system is ordered. The spontaneous magnetization $M_0 \propto |\delta|^\beta$ with $\beta = (3 - \sqrt{5})/2 \approx 0.38$, while for small applied fields H the magnetization $M(H) \propto M_0[1 + \mathcal{O}(H^{2|\delta|}\delta\ln H)]$; the susceptibility is infinite with a continuously variable exponent. The mean correlation function $\overline{\langle S^z_{fj}S^z_{fj+x}\rangle} - M_0^2 \propto |\delta|^{2\beta}(\xi/x)^{5/6}e^{-x/\xi}\exp[-3(\pi x/\xi)^{1/3}]$ for $x \gg \xi$ and where the averaging is over $\rho(h)$ [7].

Further lowering J, we reach the true phase transition Eq. (6). The correlation length is infinite, the magnetization $M(H) \propto \overline{|\ln H|^{-\beta}}$ for small H, and the mean correlation function $\overline{\langle S^z_{fj}S^z_{fj+x}\rangle} \propto x^{-\beta}$.

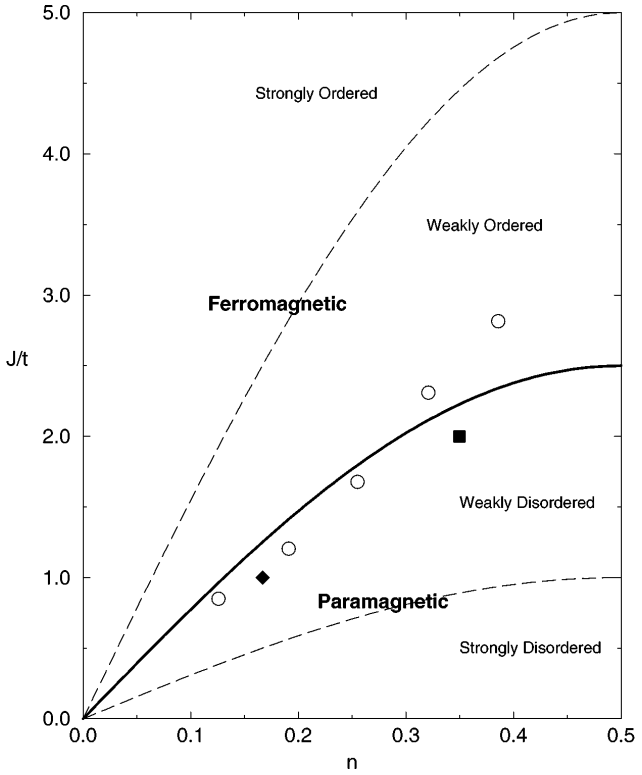

FIG. 1. Ground-state phase diagram of the 1D KLM. The solid (critical) line is from Eq. (6) with $4\pi^2\mathcal{N}^2(\alpha)/a\mathcal{J}_1(\alpha)$ used as a fitting parameter to numerically determined points: the square is density-matrix renormalization-group data of a 75 site chain from Ref. [4]; the diamond is the quantum Monte Carlo data for a 24 site system from Ref. [6]; open circles are the exact numerical diagonalization data for the eight site chain from Ref. [5]. The dashed lines separate conventional strongly ordered (FM)/disordered (PM) phases from their weak (Griffiths phase) counterparts.

Immediately below the critical line ($\delta > 0$), the system presents a weakly disordered Griffiths phase. The remaining clusters occupy a small fraction of the system length but "think" that they are still in the ordered phase; their magnetization δ^β per unit length is identical to M_0 of the weakly ordered phase. These remaining rare clusters dominate the low-energy physics. The magnetization $M(H) \propto \delta^\beta\{H^{2\delta}[\delta\ln(1/H) + \mathrm{const}] + \mathcal{O}[H^{4\delta}\delta\ln(1/H)]\}$; thus $M(H)$ has a power law singularity with a continuously variable exponent 2δ; as in the weakly ordered phase the susceptibility is *infinite*. The mean correlation function decays less rapidly than in the ordered phase, but takes the same form $\overline{\langle S^z_{fj}S^z_{fj+x}\rangle} \propto \delta^{2\beta}(\xi/x)^{5/6}e^{-x/\xi}\exp[-3/2(\pi x/\xi)^{1/3}]$ for $x \gg \xi = 1/\delta^2$. According to H_{crit}, the weakly disordered Griffiths phase extends down to $J = 0$. However, as the disorder increases, the third term in H_{eff} is no longer negligible. At very low J, the last two terms in H_{eff} will dominate; this corresponds to free spins in a field with dominant correlations at $2k_F$ of the conduction band, and is responsible for the observed peak in the f-spin structure factor [4–6]. No clusters remain. This strongly disordered conventional PM phase is indicated schematically in Fig. 1.

In summary we have derived an effective Hamiltonian for the f spins in the 1D KLM which reproduces all the behavior seen in numerical simulations in the intermediate to weak coupling regime: (i) H_{eff} presents a FM phase at intermediate coupling due to "forward" scattering by delocalized CEs, and is consistent with known limiting behavior [2,3]. (ii) As J is lowered this phase is gradually disordered due to spin-flip interactions between the CEs and the f spins. A sharp quantum order-disorder transition occurs to a PM phase at a critical coupling given in Eq. (6). (iii) The backscattering interactions leave a residue correlation at $2k_F$ in the f spins at weak coupling.

This work was supported by the Australian Research Council.

[1] See, for example, P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Condens. Matter Phys. **12**, 99 (1986).
[2] M. Sigrist, H. Tsunetsugu, and K. Ueda, Phys. Rev. Lett. **67**, 2211 (1991); see also M. Sigrist, K. Ueda, and H. Tsunetsugu, Phys. Rev. B **46**, 175 (1992).
[3] M. Sigrist, H. Tsunetsugu, K. Ueda, and T. M. Rice, Phys. Rev. B **46**, 13 838 (1992).
[4] S. Moukouri and L. G. Caron, Phys. Rev. B **52**, R15 723 (1995).
[5] H. Tsunetsugu, M. Sigrist, and K. Ueda, Phys. Rev. B **47**, 8345 (1993); see also K. Ueda, T. Nishino, and H. Tsunetsugu, Phys. Rev. B **50**, 612 (1994).
[6] M. Troyer and D. Würtz, Phys. Rev. B **47**, 2886 (1993).
[7] Daniel S. Fisher, Phys. Rev. Lett. **69**, 534 (1992); Phys. Rev. B **51**, 6411 (1995).
[8] S. Tomonaga, Prog. Theor. Phys. **5**, 544 (1950).
[9] M. Schick, Phys. Rev. **166**, 404 (1968).
[10] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[11] J. Voit, Rep. Prog. Phys. **57**, 977 (1994).
[12] V. J. Emery and S. Kivelson, Phys. Rev. B **46**, 10 812 (1992); O. Zachar, S. A. Kivelson, and V. J. Emery, Phys. Rev. Lett. **77**, 1342 (1996).
[13] S. Moukouri, L. Chen, and L. G. Caron, Phys. Rev. B **53**, R488 (1996).
[14] G. B. Honner and M. Gulácsi (unpublished).
[15] See, for example, A. A. Abrikosov and S. I. Moukhin, J. Low Temp. Phys. **33**, 207 (1978).
[16] R. B. Griffiths, Phys. Rev. Lett. **23**, 17 (1969).