

Impurity effects on the flux phase quantum-critical-point scenario

E. CAPPELLUTI(*) and R. ZEYHER

*Max-Planck-Institut für Festkörperforschung
Heisenbergstr. 1, 70569 Stuttgart, Germany*

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Abstract. – Impurity substitution of Zn in La-214 and (Y, Ca)-123 high- T_c superconductors suppresses T_c but does not affect appreciably the onset of the pseudogap phase in the underdoped region nor optimal doping or the position of the inferred quantum critical point. Based on a $1/N$ expansion of the t - J model we explain these findings as well as the similar dependence on a magnetic field in terms of a quantum-critical-point scenario where a flux phase causes the pseudogap.

The quantum-critical-point scenario [1–3] represents a popular frame to discuss the phase diagram of high- T_c oxides. By suppressing superconductivity by strong magnetic fields it has been found experimentally [4] that there exists a critical hole doping δ^{QCP} at zero temperature which separates a metallic state at larger dopings from an insulating state at lower dopings. Strong fluctuations of the order parameter related to the insulating phase are thought to suppress the density of states for $\delta < \delta^{\text{QCP}}$ leading to the pseudogap features in the underdoped region and to be instrumental for superconductivity around δ_c and, at higher temperatures, for the anomalous properties of the normal state in these systems.

The microscopic nature of the order parameter of the insulating phase and its fluctuations are presently not clear. One obvious choice is antiferromagnetism [1] which occurs at $T = 0$ as long-range ordered phase at zero and small dopings. The corresponding zero-temperature critical point, however, corresponds to a much smaller doping value than the observed one, $\delta^{\text{QCP}} \sim 0.17$. A reasonable large δ^{QCP} has been obtained in ref. [2] for a scenario with an incommensurate charge density wave (ICDW). In this approach the pseudogap features are not directly related to the ICDW order parameter but rather connected to strong d -wave superconducting fluctuations sustained by ICDW precursors. Related approaches include preformed Cooper pairs where phase coherence is achieved below T_c [5] or RVB spinon pairing [6] and

(*) Present address: Dipartimento di Fisica, Università di Roma I “La Sapienza”, P.le Aldo Moro 2, 00184 Roma, Italy.

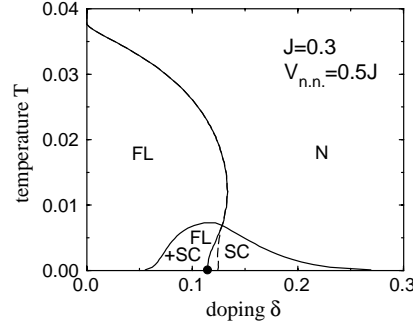


Fig. 1 – Phase diagram of the t - J - V model (see text) taking into account the normal (N), superconducting (SC), and the flux phase (FL) as well as the coexisting state of superconductivity and flux phase (FL+ SC). The normal state-flux phase transition ends in a $T = 0$ quantum critical point at $\delta^{\text{QCP}} \simeq 0.115$. The dashed line represents the instability towards the flux phase in the superconducting state.

the π -flux phase [7], where charge coherence is obtained by Bose condensation of holons. A different proposal has been made in ref. [8]. Based on a $1/N$ expansion for the t - J model the quantum critical point was identified with a transition from the normal to a d -wave flux state occurring near the observed δ^{QCP} for realistic parameters. In this approach optimal doping is determined by the onset of the flux phase and the phase diagram in the underdoped region is characterized by the competition between the flux and superconducting order parameters both having d -wave symmetry.

Recently, several experimental results have been published which may be able to confirm or to rule out some of the above approaches. Measurements of NMR spin lattice relaxation rates in the presence of magnetic fields up to ~ 15 T did not yield appreciable changes for the onset temperature T^* of the pseudogap phase, whereas the superconducting T_c was reduced by about 8 K [9]. A strong suppression of T_c and, at the same time, no change in the pseudogap was previously reported in Zn-doped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ [10]. High-resolution photoemission [11], electronic Raman spectroscopy [12], NMR [13] and heat capacity data [14, 15] show that T^* does not merge with T_c in the overdoped regime, but vanishes near optimal doping. These findings indicate that the pseudogap and the superconductivity are different phenomena and not related to the same order parameter. Furthermore, it has been found experimentally [16] that the lowering of the T_c curves in Zn-doped $\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2\text{Cu}_3\text{O}_7$ ((Y, Ca)-123) and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (La-214), is concentrated around optimal doping and that the optimal doping itself is not shifted. It is the purpose of this letter to investigate the influence of impurity scattering and magnetic fields on the phase diagram calculated in ref. [8] and to compare the results with the above experimental findings.

We consider a t - J - V model with N degrees of freedom per lattice site on a square lattice. Its Hamiltonian can be written in terms of Hubbard's X -operators as [8]

$$\begin{aligned}
 H = & -\frac{t}{N} \sum_{\substack{\langle ij \rangle \\ p=1 \dots N}} X_i^{p0} X_j^{0p} + \frac{J}{4N} \sum_{\substack{\langle ij \rangle \\ p,q=1 \dots N}} X_i^{pq} X_j^{qp} - \\
 & -\frac{J}{4N} \sum_{\substack{\langle ij \rangle \\ p,q=1 \dots N}} X_i^{pp} X_j^{qq} + \sum_{\substack{ij \\ p,q=1 \dots N}} \frac{V_{ij}}{2N} X_i^{pp} X_j^{qq}. \quad (1)
 \end{aligned}$$

The internal labels $p, q \dots$ consist of a spin label distinguishing spin-up and spin-down states and a flavor label counting $N/2$ identical copies of the original orbital. $\langle ij \rangle$ denotes nearest-neighbor sites. The first three terms represent the t - J Hamiltonian, the last term a screened Coulomb interaction appropriate for two dimensions and taken from ref. [17]. In the following we express all energies in units of t . The strength of the Coulomb interaction will be characterized by its value between nearest-neighbor sites $V_{\text{n.n.}}$. In the limit of large N , the interactions become purely instantaneous and H can be diagonalized analytically. In the absence of impurity scattering, the coexistence state of superconductivity and a staggered (π, π) flux phase can be obtained from a Nambu representation with 4 states yielding four electronic bands with dispersion [8]

$$\pm E_{\pm}(\mathbf{k}) = \pm \sqrt{[\xi(\mathbf{k}) \pm \tilde{\mu}]^2 + \Delta(\mathbf{k})^2}, \quad (2)$$

where

$$\xi(\mathbf{k}) = \sqrt{\epsilon(\mathbf{k})^2 + \phi(\mathbf{k})^2}. \quad (3)$$

Here the momenta \mathbf{k} are restricted to the new Brillouin zone which is one half of the original one. $\tilde{\mu}$ is a renormalized chemical potential, $\phi(\mathbf{k})$ the flux order parameter, $\Delta(\mathbf{k})$ the superconducting gap, and $\epsilon(\mathbf{k})$ the one-particle energies in the normal state. Both order parameters have d -wave symmetry: $\phi(\mathbf{k}) = \phi[\cos(k_x) - \cos(k_y)]$, $\Delta(\mathbf{k}) = \Delta[\cos(k_x) - \cos(k_y)]$. They are determined by the self-consistent set of equations:

$$\phi(\mathbf{k}) = \frac{1}{2N_c} \sum_{\mathbf{p}} J(\mathbf{k} + \mathbf{p}) \eta_{\phi}(\mathbf{p}), \quad (4)$$

$$\Delta(\mathbf{k}) = \frac{1}{2N_c} \sum_{\mathbf{p}} [J(\mathbf{k} + \mathbf{p}) - V_{\text{n.n.}}(\mathbf{k} + \mathbf{p})] \eta_{\Delta}(\mathbf{p}), \quad (5)$$

where

$$\eta_{\phi}(\mathbf{k}) = \frac{\phi(\mathbf{k})}{\xi(\mathbf{k})} \left\{ \frac{\xi(\mathbf{k}) + \tilde{\mu}}{2E_+(\mathbf{k})} \tanh \left[\frac{E_+(\mathbf{k})}{2T} \right] + \frac{\xi(\mathbf{k}) - \tilde{\mu}}{2E_-(\mathbf{k})} \tanh \left[\frac{E_-(\mathbf{k})}{2T} \right] \right\}, \quad (6)$$

$$\eta_{\Delta}(\mathbf{k}) = \frac{\Delta(\mathbf{k})}{2E_+(\mathbf{k})} \tanh \left[\frac{E_+(\mathbf{k})}{2T} \right] + \frac{\Delta(\mathbf{k})}{2E_-(\mathbf{k})} \tanh \left[\frac{E_-(\mathbf{k})}{2T} \right]. \quad (7)$$

The resulting phase diagram, calculated using $J = 0.3$ and $V_{\text{n.n.}} = 0.5J$, is shown in fig. 1. Disregarding superconductivity, the second-order normal-state-flux phase transition line ends in a quantum critical point, denoted by the black dot, at $\delta^{\text{QCP}} \sim 0.115$. We find the maximum of T_c at essentially the same doping because of the strong competition between flux and superconducting phase [8], and also that the flux phase instability is only slightly shifted by superconductivity (dashed line).

Now we are going to investigate how the phase diagram in fig. 1 is affected by impurity scattering. In the simplest approximation, the effects of impurities in the normal state can be taken into account by introducing a renormalized frequency [18]

$$i\tilde{\omega}_n = i\omega_n + i\Gamma \frac{\omega_n}{|\omega_n|}, \quad (8)$$

where Γ is a scattering rate, here used as a free parameter proportional to the impurity concentration. Throughout the flux phase the self-energy due to impurity scattering is still diagonal in the 4×4 Nambu representation because the flux order parameter does not couple

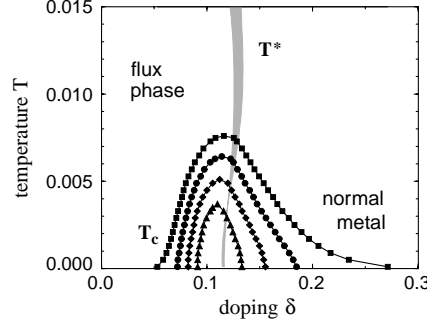


Fig. 2 – Solid lines: suppression of T_c by impurity scattering, calculated with the scattering rates $\Gamma = 0$ (squares), $2 \cdot 10^{-3}$ (circles), $4 \cdot 10^{-3}$ (diamonds), and $6 \cdot 10^{-3}$ (triangles). Grey region: corresponding variation of the transition temperature T^* to the flux state.

to the impurities. The constant Γ in eq. (8) could be improved in a deeper analysis considering effects due to the proximity of the Van Hove singularity [19]. However, the interesting doping region for superconductivity is in our model not at all correlated with the Van Hove singularity. As a matter of fact, the chemical potential for $\delta \sim 0.1$ is quite far away from the Van Hove singularity, which is at $\delta = 0$ in our model. In this situation the band can be assumed in a good approximation to be structureless and Γ as a constant, even in the case of strong potential scattering [19]. Experimentally it is known that non-magnetic impurities such as Zn and Al induce local moments on neighboring Cu sites [10,20]. Both in a d -wave flux phase and a d -wave superconductor random local magnetic moments lead only to renormalizations of the frequency. As a result they contribute additively to Γ in eq. (8) and thus can be accounted for by a proper choice for Γ . It also has been argued [20] that strong potential scattering near the unitary limit is much more important for the reduction of T_c than the scattering from induced magnetic moments.

The occupation number f_Γ of an electronic state with energy ϵ in the presence of impurities reads

$$\begin{aligned} f_\Gamma \left(\frac{\epsilon}{T} \right) &= T \sum_n \frac{e^{i\omega_n 0^+}}{i\tilde{\omega}_n - \epsilon} \\ &= \frac{1}{2} + \frac{1}{2\pi} \text{Im} \left[\psi \left(\frac{1}{2} - i \frac{\epsilon + i\Gamma}{2\pi T} \right) - \psi \left(\frac{1}{2} + i \frac{\epsilon - i\Gamma}{2\pi T} \right) \right], \end{aligned} \quad (9)$$

where ψ denotes the digamma function. In the limit of zero impurity concentration $\Gamma \rightarrow 0$ and $f_\Gamma(\epsilon/T)$ reduces to the usual Fermi function $f(x) = 1/(e^x + 1)$. In a similar way, we also define a function tanh_Γ by

$$\text{tanh}_\Gamma \left(\frac{\epsilon}{2T} \right) = \frac{1}{2} \left[f_\Gamma \left(-\frac{\epsilon}{T} \right) - f_\Gamma \left(\frac{\epsilon}{T} \right) \right]. \quad (10)$$

For the determination of the superconducting critical temperature T_c , the self-consistent set of gap equations can be linearized with respect to $\Delta(\mathbf{k})$. The resulting equations are again given by eqs. (4)-(7) if the function \tanh is everywhere replaced by the function tanh_Γ , defined in eq. (10). The solid lines in fig. 2 show numerical results for T_c as a function of doping δ for different scattering rates Γ , using $J = 0.3$ and $V_{\text{n.n.}} = 0.5J$. These curves illustrate the suppression of T_c with increasing scattering rates $\Gamma = 0, 2 \cdot 10^{-3}, 4 \cdot 10^{-3}$, and

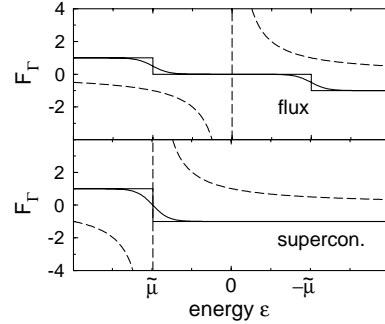


Fig. 3 – Numerator (solid lines) and denominator (dashed line) of $F_\Gamma(\epsilon)$, eq. (12), in the case of the flux instability of the normal state (upper panel). The discontinuous and continuous solid lines refer to zero and non-zero effective temperature, respectively. For comparison, the lower panel shows the corresponding quantities in the case of a superconducting instability.

$6 \cdot 10^{-3}$. The corresponding changes in T^* , determining the phase boundary between the normal state and the flux state, are depicted in fig. 2 by the grey region. The chosen values for Γ correspond roughly to $\Gamma \simeq 1.0T_c$ at optimal doping, and to $\Gamma \simeq 1.5T_c$ in the strongly underdoped region, interpolating between the weak- and the strong-coupling regimes. One important result of fig. 2 is that the flux phase boundary $\delta^{\text{FL}}(T)$ is only slightly shifted by impurities, in spite of the strong suppression of the superconducting critical temperature. In particular, the zero-temperature limit of δ^{FL} , $\delta^{\text{FL}}(0)$, is almost completely independent of the impurity scattering rate. Since in our approach the maximum of T_c as a function of doping is essentially determined by $\delta^{\text{FL}}(0)$, this means that the $T_c(\delta)$ curves shrink to $\delta^{\text{FL}}(0)$ with increasing scattering rate which is a characteristic feature of fig. 2. Interpreting fig. 2 in terms of a quantum-critical-point scenario means that the corresponding critical doping δ^{QCP} is given by $\delta^{\text{FL}}(0)$ and that δ^{QCP} is almost completely independent of the impurity scattering rate. The curves in fig. 2 are in excellent agreement with the corresponding experimental curves in Zn doped (Y, Ca)-123 and La-214, given in fig. 2 of ref. [16].

We can gain further insight into our results by the following analysis. We first notice that, at least for the above values of Γ , impurity scattering effects lead to an additional smearing of the occupation number in eq. (9) which can be simulated in a very good approximation by an effective temperature:

$$f_\Gamma\left(\frac{\epsilon}{T}\right) \simeq f\left(\frac{\epsilon}{T+\Gamma}\right). \quad (11)$$

As a consequence, the flux phase instability in the presence of impurities is roughly determined by $\delta_\Gamma^{\text{FL}}(T) \simeq \delta^{\text{FL}}(T+\Gamma)$. But δ^{FL} is very weakly dependent on T until $T \sim \tilde{\mu}$, so that the $T=0$ quantum critical point is not expected to be shifted as long as $\Gamma \lesssim \tilde{\mu}$ holds.

In order to understand better why $\delta^{\text{FL}}(T)$ is almost independent of T for $\Gamma \lesssim \tilde{\mu}$, we consider the flux phase susceptibility $\chi(T, \Gamma, \delta)$. The instability line $\delta^{\text{FL}}(T)$ is determined in general by the equation: $1 = J\chi(T, \Gamma, \delta)$, where the dependence of the susceptibility on temperature and impurities is given by the factor [8]

$$F_\Gamma(\epsilon) = \frac{f_\Gamma[(\epsilon - \tilde{\mu})/T] - f_\Gamma[(-\epsilon - \tilde{\mu})/T]}{\epsilon}. \quad (12)$$

A sketch of the numerator and denominator of F_Γ is given in fig. 3. Continuous and discontinuous solid lines represent the numerator for $\Gamma \neq 0$ and $\Gamma = 0$, respectively, the dashed line

the denominator. Due to the weak variation of the denominator around $\tilde{\mu}$ and $-\tilde{\mu}$, it is clear that this factor is only slightly affected by a possible smearing due to finite temperatures or impurity concentrations, as long as $T + \Gamma \lesssim \tilde{\mu}$ holds. Things are different in the case of the superconducting susceptibility. Here the divergence of the denominator coincides with the jump in the numerator, so that even a small smearing leads to a strong change in χ and a large suppression of T_c .

We would like to mention that a charge-density-wave susceptibility would contain a similar factor as in eq. (12), so that also in this case impurities will not affect substantially the function F_Γ . However, the CDW order parameter has the symmetry of the underlying lattice, *i.e.*, *s*-wave symmetry. Impurities couple in this case directly to the order parameter and the self-energy due to impurity scattering also acquires non-diagonal elements in addition to the diagonal ones described by eq. (8). As a result, one expects that the charge-density wave state is sensitive to impurities and the corresponding quantum critical point and optimal doping would be shifted by the impurities, in disagreement with ref. [16].

We have considered throughout our analysis a (π, π) flux phase and its competition with superconductivity. In ref. [21] it was shown that there is a continuous transition line in the T - δ plane from a commensurate to an incommensurate flux state at low temperatures (the term “commensurate” is here used with respect to the lattice periodicity and not, as in ref. [22], with respect to the electronic filling). Taking the incommensurability into account the largest onset of the flux phase as a function of doping occurs now at $T = 0$ with a critical doping $\delta^{\text{QCP}} \sim 0.135$. However, the boundaries in the phase diagram and, in particular, the competition between flux and superconducting phases are not much changed by allowing for the incommensurability of the flux phase. Disregarding superconductivity we also have studied the influence of impurities on the boundary between an incommensurate flux and the normal phase. The resulting width in T^* for the scattering rates used in fig. 2 is very similar to that shown in this figure for the commensurate case. In particular, the change of the critical doping at $T = 0$ was for all Γ 's smaller than 0.01 showing that our fig. 2 calculated for the commensurate case is also valid in the incommensurate case in a very good approximation. Also the simplified arguments based on fig. 3 for the robustness of the flux state in contrast to the superconducting state with respect to impurities still apply. The finiteness of the chemical potential $\tilde{\mu}$ reflects the fact that one-particle states which are also not exactly degenerate in energy are involved in forming the flux state. This means that finite difference energies $|\epsilon(\mathbf{k}) - \epsilon(\mathbf{k} + \mathbf{Q})|$ (\mathbf{Q} is the wave vector of the flux phase) associated with a large phase space are important which can be characterized by a typical energy $2\tilde{\mu}$. This explains why both the commensurate and the incommensurate flux phase behave in a very similar way with respect to impurities.

Our proposed scenario of a flux quantum critical point is also consistent with the NMR measurements of ref. [9]. In that paper, a magnetic field $H = 14.8$ T was shown to yield a net reduction of the superconducting critical temperature of $\Delta T_c = 7.8$ K but no corresponding decrease of the pseudogap temperature T^* within the experimental uncertainty of 2 %. In our theory the pseudogap and the superconductivity arise from two different mechanisms, so that a significant reduction of T_c is possible in the absence of a corresponding reduction of T^* . The predominant effect of a magnetic field on the superconducting phase is a reduction of T_c in order to balance the free magnetic energy related to the Meissner effect. The decrease of T_c is linear in H for $H \ll H_c$ (H_c being the critical magnetic field), so that the reduction in T_c is quite effective even for small magnetic fields. On the other hand, the effect of a magnetic field on the flux phase is mainly due to the Zeeman splitting $\Delta E = g\mu_B H$, where g and μ_B are the g factor and the Bohr magneton, respectively. This energy is about 20 K for $H = 14.8$ T [9], and thus much smaller than the width of the electronic band. If we generalize our order

parameter ϕ in the presence of a magnetic field via $\phi \rightarrow \phi = [\phi_{\uparrow}(\tilde{\mu} - \Delta E) + \phi_{\downarrow}(\tilde{\mu} + \Delta E)]/2$, we obtain an effective susceptibility given by $\chi = [\chi_{\uparrow}(\tilde{\mu} - \Delta E) + \chi_{\downarrow}(\tilde{\mu} + \Delta E)]/2$. The Zeeman splitting $\Delta E = 20$ K is much smaller than the energy scale set by the bandwidth $W \approx 0.5$ eV, so that we expect a negligible effect on the flux instability. Moreover, the shift of T_c will be only of order H^2 in the magnetic field.

We have checked the above arguments by calculating explicitly the change in the instability from the normal to the flux state in the presence of a Zeeman splitting $\Delta E = 20$ K, corresponding to $\Delta E = 6 \cdot 10^{-3}t$ with $t = 0.3$ eV. We find a shift in doping of the $T = 0$ quantum critical point of about 4%, which is quite small. This shift disappears with increasing temperature because of thermal smearing which makes the Zeeman splitting ineffective.

In conclusion, we have analyzed the effects of impurity scattering on the flux phase and on its interplay with superconductivity within the framework of a quantum-critical-point scenario. We have found that the transition between the flux and the normal phase is essentially unaffected by impurities and magnetic fields, in very good agreement with the experimental data. This is especially true at zero temperature where we identify the quantum critical point with the transition between the normal and the (incommensurable) flux state. We also pointed out that a charge density wave as the origin of the pseudogap phase would directly couple to impurities in contrast to the flux order parameter and thus be much more sensitive to impurities.

REFERENCES

- [1] MONTHOUX P. and PINES D., *Phys. Rev. B*, **50** (1994) 16015; BARZYKIN V. and PINES D., *Phys. Rev. B*, **52** (1995) 13585.
- [2] CASTELLANI C., DI CASTRO C. and GRILLI M., *Phys. Rev. Lett.*, **75** (1995) 4650; *Z. Phys. B*, **103** (1997) 137.
- [3] VARMA C. M., *Phys. Rev. B*, **55** (1997) 14554.
- [4] BOEBINGER G. S. *et al.*, *Phys. Rev. Lett.*, **77** (1996) 5417.
- [5] EMERY V.J. and KIVELSON S.A., *Nature*, **374** (1995) 434.
- [6] TANAMOTO T., KOHNO H. and FUKUYAMA H., *J. Phys. Soc. Jpn.*, **63** (1994) 2739.
- [7] WEN X.-G. and LEE P.A., *Phys. Rev. Lett.*, **76** (1996) 503.
- [8] CAPPELLUTI E. and ZEYHER R., *Phys. Rev. B*, **59** (1999) 6475.
- [9] GORNY K. *et al.*, *Phys. Rev. Lett.*, **82** (1999) 177.
- [10] ALLOUL H. *et al.*, *Phys. Rev. Lett.*, **67** (1991) 3140.
- [11] INO A. *et al.*, *Phys. Rev. Lett.*, **79** (1997) 2101; **81** (1998) 2124.
- [12] NAEINI J. G. *et al.*, *Phys. Rev. B*, **59** (1999) 9642.
- [13] WILLIAMS G. V. M. *et al.*, *Phys. Rev. Lett.*, **78** (1997) 721.
- [14] LORAM J. W. *et al.*, *Physica C*, **282-287** (1997) 1405.
- [15] WILLIAMS G. V. M., TALLON J. L. and LORAM J. W., *Phys. Rev. B*, **58** (1998) 15053.
- [16] TALLON J. L. *et al.*, *Phys. Rev. Lett.*, **79** (1997) 5294.
- [17] BECCA F. *et al.*, *Phys. Rev. B*, **54** (1996) 12443.
- [18] ABRIKOSOV A. A. and GORKOV L. P., *Sov. Phys. JETP*, **12** (1961) 1243.
- [19] FEHRENBACHER R., *Phys. Rev. Lett.*, **77** (1996) 1849.
- [20] ISHIDA K., KITAOKA Y., YAMAZOE K. and ASAYAMA K., *Phys. Rev. Lett.*, **76** (1996) 531.
- [21] CAPPELLUTI E. and ZEYHER R., *Physica C*, **312** (1999) 313.
- [22] LEDERER P., HASEGAWA Y. and T. M. RICE, *Phys. Rev. Lett.*, **63** (1989) 1519.